Scientific paper

Spectral Properties of Novel 1,3-oxazol-5(4*H*)-ones With Substituted Benzylidene and Phenyl rings

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Abstract

In the present work, five novel (4*Z*)-4-benzylidene-2-phenyl-1,3-oxazol-5(4*H*)-ones (azlactones) were investigated by the infra-red (IR) and nuclear magnetic resonance spectroscopy (NMR) of the ^{1}H and ^{13}C nuclei. The spectral properties of the oxazolone ring were monitored with respect to the substituents at the benzylidene and phenyl rings. The compounds were prepared by the Erlenmeyer–Plöchl synthesis from the respective substituted aldehydes and hippuric acid. The IR absorption spectra, measured in chlorophorm, showed a clear splitting of the vibration band in the region characteristic for the carbonyl stretching vibration. This splitting was attributed to the Fermi resonance and the unperturbed wavenumbers of the carbonyl stretching bands were calculated. The chemical shifts of the carbons of the oxazolone ring were assigned. The influence of substituents on spectral properties was demonstrated and discussed. It was found that the oxazolone molecule constitutes an extended π-electron system, with an efficient transmission of electron effects.

Keywords: (*Z*)-4-benzylidene-2-phenyl-1,3-oxazol-5(4*H*)-one, substituent effect, C=O stretching vibration, Fermi resonance

1. Introduction

4-Benzylidene-2-phenyl-1,3-oxazol-5(4*H*)-ones (azlactones) are compounds with a significant synthetic potential and several biological and technological applicatons.[1–6] The compounds can be, for example, used as inhibitors of the enzyme activity or as fluorescent sensors.[3,6] In addition, the oxazolone molecule serves as a general template for the stereoselective syntheses of amino acids and heterocyclic scaffolds.[2]

The structure of the compounds was investigated by several authors.[7–9] It has been found that the stable configuration is *cis* (*Z*) with respect to the exocyclic C=C double bond. The absorption of the electromagnetic energy induces the transition to the *trans* (*E*) isomer. The *E* form, however, is metastable and the reverse transformation to the *Z* configuration occurs through the photoactivation.[10] The compounds posses an extended π-conjugation system. Their properties are sensitive to substituent effects. The effect of substituents on the biological activity,[3,4] the rate of ring-opening reactions,[11,12] and spectral properties were demonstrated.[13]

In solution, the hetero ring is unstable, opens easily and the respective fluorescence quantum yields are relatively low. In the solid state, however, the ring is stable and the quantum yields are enhanced.[14–16] The significant photochemical and photophysical applications are, therefore, expected for the oxazolone molecules in the solid state, for instance, when embedded in a polymer matrix.[14,17] The presence of weak van der Waals interactions and the lack of hydrogen bonds causes the molecules to pile up in the same direction and crystallize in noncentrosymmetric structures.[5] The study of substituted 4-benzylidene-2-phenyl-1,3-oxazol-5(4*H*)-ones showed that the second order harmonic generation (SHG) values of 4-benzo-[1,3]dioxol-5-ylmethylene-2-phenyloxazol-5(4*H*)-one were significantly higher compared to 4-(3,4-dimethoxy-benzylidene)-2-phenyloxazol-5(4*H*)-one.[18] This was attributed to a different way of piling up the molecular columns and to the resulting overlapping of the rings between the molecules in the π–π stacks. The relationship between the structure and the SHG efficiencies suggested that the dominant role was played by the expansion of the delocalized range of π-electrons by the electron donor group rather than the acceptor at the *para* position of the benzylidene ring. This observation has led to an intensive investigation of the oxazolones having electron donor

substituents and especially the alkyloxy and alkylamino substituted compounds have received a lot of consideration in recent years.[18–20]

In the present work, we aim to investigate the spectral properties of five novel oxazolone molecules in order to shed further light on substituent effects. The structure of the compounds is given in Fig. 1. The spectral properties were studied for the compounds with the butoxy and isobutoxy electron donor groups located at the *para* position of the phenyl ring. The effect of substitution was monitored by the change of substituents located at the benzylidene ring.
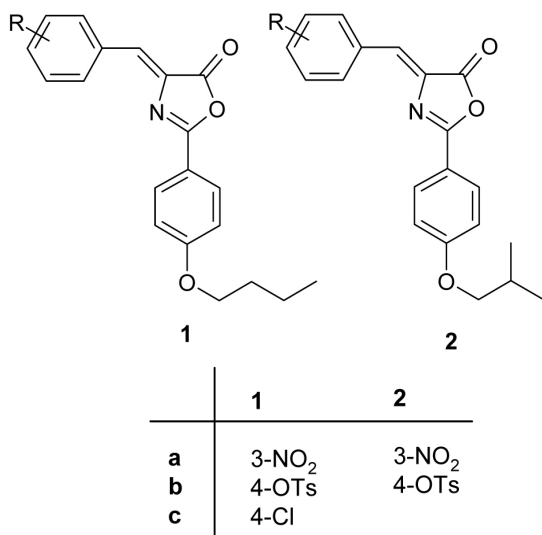

	1	**2**
a	3-NO$_2$	3-NO$_2$
b	4-OTs	4-OTs
c	4-Cl	

Fig. 1: The structure of the compounds investigated in the study. Ts stands for the tosyl group, i.e. 4-Me–C$_6$H$_4$–SO$_2$–.

2. Results and Discussion

2. 1. Stretching Frequencies of the C=O and C=N groups

1,3-Oxazol-5(4H)-ones have multiple electrophilic reaction centres for an attack of the nucleophile. In most cases, they react at the carbonyl group.[1,2,21] The nucleophilic attack often leads to a ring opening and the reaction products are, depending on the character of the nucleophi-
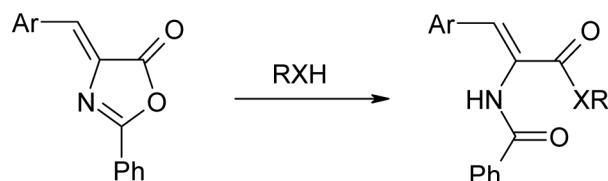

Fig. 2: Ring opening of the hetero ring by a nuclephilic attack at the carbon of the carbonyl group.

le, the respective derivatives of the 2-(R$_1$-benzoylamino)-3-(R$_2$-phenyl)acrylic acid. The reactivity of the carbonyl carbon is, therefore, of a primary interest. The reaction scheme is given in Fig. 2. The benzene rings with different substituents were denoted as Ar and Ph in this scheme.

Beside the carbonyl group, the attack of the C=N group by some nucleophiles has also been reported.[22] The charge distribution on the carbons of the hetero ring may reveal possible electrophilic reaction centres for the attack of the nucleophile. We have, therefore, calculated the atomic charges on the hetero ring's atoms for compounds **1a–c**, **2a,b**. The optimum configurations and conformations for the molecules in vacuum were calculated using the semiempirical AM1 Hamiltonian within the program package HYPERCHEM 7.0.[23] The data are given in Table 2. The results show that the net charge of carbon C$_5$ (carbon of the carbonyl group) is about two-times larger than the charge of carbon C$_2$. The charge of carbon C$_2$, however, is greatly influenced by the character of substituent at the benzylidene ring. The *m*-NO$_2$ group increases the positive charge of carbon C$_2$, which may become attractive for an attack by some nucleophiles. Although the negative effect of the nitro group is partly decreased by the presence of the alkoxy group at the *para* position of the phenyl ring, the electron withdrawing effect of this group may support the attack of the C=N group.

Table 1 Calculated net atomic charges and bond orders of 1,3-oxazol-5(4H)-ones **1a-c, 2a, b**.
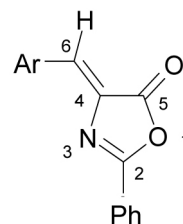
	Atomic charges		
	C$_2$	**C$_4$**	**C$_5$**
1a	0.169	–0.115	0.305
1b	0.144	–0.148	0.308
1c	0.153	–0.135	0.306
2a	0.170	–0.115	0.306
2b	0.144	–0.148	0.308

	Bond orders		
	O$_1$–C$_2$	**C$_2$–N$_3$**	**C$_5$–O$_1$**	**C$_5$=O**
1a	0.993	1.699	0.956	1.873
1b	0.990	1.720	0.955	1.861
1c	0.991	1.713	0.954	1.866
2a	0.994	1.698	0.955	1.874
2b	0.989	1.721	0.955	1.861

Another important factor is the influence of substituents on the order of the chemical bond. Calculated bond orders of chemical bonds forming the 1,3-oxazol-5(4H)-

ones **1a**–**1c** and **2a,b** are presented in Table 3. The bond orders are influenced by the electron withdrawing effect of the substituents. The *m*-NO$_2$ group at the benzylidene ring decreases the bond order of the C=N group. The influence of substituents, however, is evident also for the carbonyl group and not only for the chemical bonds forming the 5-membered heteronuclear ring. The strength of chemical bonds may be inferred from the force constant, which is proportional to the frequency of the critical vibration. We have, therefore, decided to study the stretching vibrations of the C=N and C=O groups in the liquid state.

The frequencies of the stretching vibrations were studied in CHCl$_3$ solutions. We have chosen the chlorophorm as a solvent since the solubility of the compounds in this solvent was very good. The characteristic band of the C=N group was present at 1640–1680 cm^{-1}, in line with the literature.[24] The absorption band had a high extinction coefficient and it had a simple shape with a clear, single peak maximum. The wavenumbers of the peak maximum together with the respective extinction coefficients for the compounds **1a**–**c**, **2a,b** are listed in Table 2. The intensity of the absorption band and the frequency of vibration are influenced by the character of the substituent at the benzylidene ring. Substituents with a strong electron withdrawing effect (*m*-NO$_2$) significantly decrease the intensity of the maxima (extinction coefficient).

Table 2: Wavenumbers (cm^{-1}) of the stretching vibration β of the C=N group and of the out-of-plane C–H deformation vibration ω together with the corresponding extinction coefficients (dm^3 mol^{-1} cm^{-1}).

	β(C=N)		ω(C–H)	
	ν	ε	ν	ε
1a	1659.2	642	885.2	260
1b	1656.0	699	886.4	312
1c	1654.4	796	886.4	273
2a	1659.6	588	886.4	226
2b	1656.0	699	886.4	344

The characteristic absorption band of the carbonyl group was found at 1770–1820 cm^{-1}. The shape of the absorption band, however, was not simple and consisted of a superposition of two or more overlapping single bands. We found two peak maximas – the more intense one at 1790 cm^{-1} (A) and the less intense one at 1760 cm^{-1} (B). A similar observation has also been found for other unsaturated lactones studied previously.[25] The stronger band belongs to the fundamental C=O stretching vibration. The results are presented in Fig. 3.
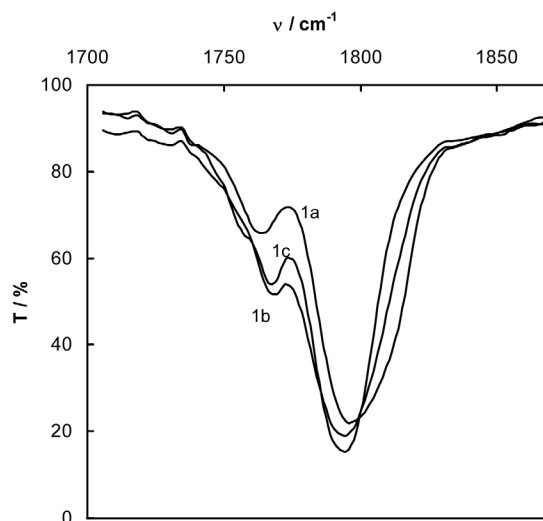
Fig. 3: The absorption bands of the compounds **1a**–**1c** in the region characteristic for the stretching vibration of the carbonyl group.

The complicated shape of the absorption band disables one to obtain the spectral characteristics precisely. Since the compounds have a characteristic deformation vibration of the C–H group ω, present in the region of ~880 cm^{-1} (Table 2), it was anticipated that the complicated shape of the absorption band came out as a result of an interaction between the first overtone of this deformation vibration mode with the fundamental stretching vibration mode of the carbonyl group. This interaction is called Fermi resonance and causes shifting of the peak maxima. It is most often observed in the spectra of lactones and can be detected by the change of solvent.[26] Based on the perturbation theory, we calculated the wavenumbers of the C=O

Table 3 IR absorption bands of oxazolones **1** and **2** in CHCl$_3$, *c* = 12.0 mmol dm^{-3}, before and after the correction for Fermi resonance; *ν* – peak wavenumber (cm^{-1}), *A* – absorbance at peak maximum, $\Delta \nu_{1/2}$ – half-peak width (cm^{-1}), *ε* – extinction coefficient (dm^3 mol^{-1} cm^{-1}), *I* – integrated intensity (dm^3 mol^{-1} cm^2), *W* – interaction coefficient

| | | Uncorrected | | | | | | | | | Corrected | | | |
| | | Branch A | | | | | Branch B | | | | | | | |
	ν	A	$\Delta \nu_{1/2}$	ε	I	ν	A	$\Delta \nu_{1/2}$	ε	I	ν_1^0	$\Delta \nu^a$	ν_2^0	$W_{1/2}$
1a	1799.2	0.597	27.3	498	5.24	1762.2	0.112	16.7	93.3	0.623	1795.4	-3.8	1766.0	11.2
1b	1794.8	0.632	26.9	527	5.66	1765.1	0.156	19.5	130	1.01	1790.3	-4.5	1769.6	10.7
1c	1793.9	0.723	21.2	603	5.10	1764.6	0.185	21.0	154	1.29	1788.0	-5.9	1770.5	11.8
2a	1799.6	0.532	29.6	443	5.23	1763.3	0.101	17.8	84.2	0.597	1795.9	-3.7	1767.0	11.0
2b	1794.6	0.666	26.4	555	5.85	1765.3	0.165	18.5	137	1.017	1790.3	-4.3	1769.6	10.4

^{a} $\Delta \nu = \nu_1^0 - \nu_A$

before the interaction. We used the relations established by Nyquist et al.[27] The results are presented in Table 3.

The shift of the peak maximum of the carbonyl absorption band due to Fermi resonance interaction (Δv) was −3.7 to −5.9 cm^{-1} depending on the character of the substituent. In order to quantify the substituent effect on the carbonyl stretching frequencies we decided to use the Hammett equation. This equation is a representation of a so-called linear free energy relationship (LFER).[28] The electron effect of the substituents was characterized by the Hammett (σ) constant.[28] The Hammett plot of the unperturbed wavenumbers of the carbonyl stretching vibration is presented in Fig. 4. The correlation was satisfactory (correlation coefficient $r = 0.9942$) and allowed us to unambiguosly relate the effect on the frequency of the stretching vibration to the electron withdrawing effect of the substituents. Since the carbonyl group is not directly bound to the benzene ring, the successful correlation shows a significant transmission of electron effects in the oxazolone ring and suggests a presence of an extended π electron system in the molecule. In order to confirm this suggestion, the transmission of the electron effects of the substituents was further investigated by the NMR spectroscopy.
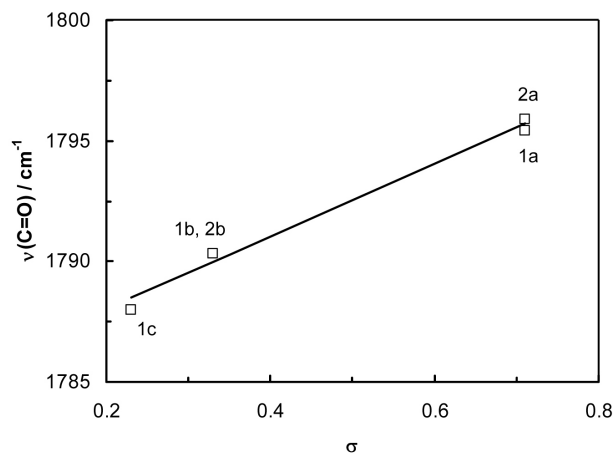
Table 4 Selected ^{13}C NMR chemical shifts (in ppm) of compounds **1** and **2**. For the numbering of atoms, see Table 1.

Cmpd	C_2	C_5	C_6
1a	164.81	166.89	125.77
1b	163.84	167.43	127.79
1c	163.84	167.76	128.29
2a	164.68	166.69	125.79
2b	163.75	167.28	127.90

The data presented in Table 4 show that substituents affected the individual chemical shifts of all carbons listed. The effect was most pronounced for carbon C_6 which was directly bound to the benzene ring bearing the variable substituent and led to an increase of the chemical shift by the *m*-NO$_2$ group. The effect of substituents was characterized by the σ constant and the individual chemical shifts could be given in a Hammett plot. The Hammett plot is presented in Fig. 5. The correlation was very good (correlation coefficient 0.9990). It can be, therefore, concluded that the chemical shifts were controlled by the electron withdrawing effect of the substituents. A very high magnitude of the slope of the Hammett plot given in Fig. 5 ($\rho = -5.32$) corresponds to a very efficient transmission of the electron effects.
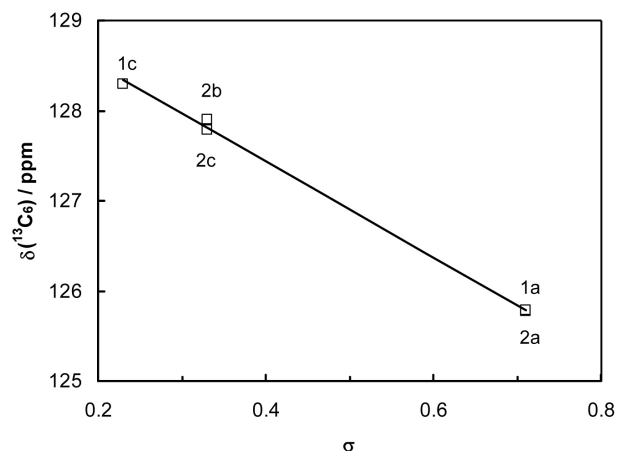

Fig. 4 The Hammett plot of the wavenumbers of the carbonyl stretching vibration.

Fig. 5: The Hammett plot of the individual chemical shifts of the carbon C_6. For the numbering of atoms, see Table 1.

2. 2. Chemical Shifts of Carbons of the Oxazolone Ring

The NMR spectra of the ^{1}H and ^{13}C nuclei were measured for saturated chlorophorm solutions. The individual chemical shifts of carbons and protons were assigned using the advanced correlation techniques DQF ^{1}H, ^{1}H COSY, APT, DEPT and ^{1}H–^{13}C HMQC.[29] This procedure allowed for an unambiguos assignment of most chemical shifts. The individual chemical shifts of the carbons of the oxazolone ring are presented in Table 4.

The chemical shifts of the hetero ring's carbons (C_2 and C_5) could be correlated with the Hammett constants as well. The efficiency of the electron effect transmission, given by the slope, was smaller. The correlation between individual chemical shifts of the carbons of the oxazolone ring is given in Fig. 6. The chemical shifts of carbon C_6 literally influence the chemical shifts of the carbons of the hetero ring. From Fig. 6 it is also apparent that the transmission of the electron effects causes an increasing chemical shift of the carbon C_5 (carbon of the C=O group) and decreasing chemical shift of carbon C_2 (carbon of the C=N group). Since the chemical shift is related to the

electron density around a nucleus, the transmission of the electron effects may, in turn, influence the relative reactivity of the C=O and C=N groups towards a nucleophilic attack. It will be a task for a future study to investigate the attack of the electrophilic centre of the compounds in the ring opening reactions.
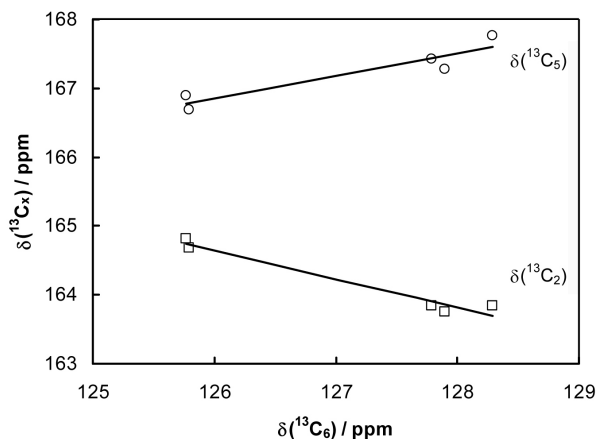
Fig. 6: The correlation of individual chemical shifts of carbons C_2 and C_5 of the oxazolone ring. For the numbering of atoms, see Table 1.

3. Conclusion

In the present study, we have investigated five novel substituted (4*Z*)-4-benzylidene-2-phenyl-1,3-oxazol-5(4*H*)-ones by IR and NMR spectroscopy in chlorophorm solutions in order to demonstrate and understand the substituent effect on spectral properties. The absorption bands of the carbonyl stretching vibration showed a clear splitting. This effect was attributed to a Fermi resonance interaction between the first overtone of a deformation vibration of the C–H group and a fundamental stretching mode of the C=O group. The unperturbed frequencies were calculated based on the relations resulting from the perturbation theory.

The frequencies of the stretching vibrations of the C=N and C=O group were found to be significantly influenced by substituent effects. A successful correlation between the wavenumbers of the carbonyl group and Hammett substituent constants was found. This result shows the control of spectral properties by the electron withdrawing/donating effect of the substituents. The transmission of the electron effects in the oxazolone ring was further investigated by the ^{13}C NMR spectroscopy. Successful Hammett plots were found for the chemical shifts of the carbon directly bound to the benzene ring bearing the variable substituent and also for the carbons of the hetero ring. These results suggest a presence of an extended π electron system in the oxazolone molecule. The electron withdrawing groups were found to have an opposite effect

on the individual chemical shifts of the carbons C_2 and C_5 of the oxazolone ring. It can be suggested that the relative reactivity of the electrophilic centres of the C=N and C=O groups towards an attack of a nucleophile shall be different for different substituents. It will be a task for a future study to investigate the rate and mechanism of the ring opening reactions of the substituted compounds.

4. Experimental

(4*Z*)-4-(Substituted benzylidene)-2-(substituted phenyl)-1,3-oxazol-5(4*H*)-ones were prepared by the cyclodehydration–condensation of the appropriate aldehyde and hippuric acid in dry acetic anhydride catalysed by acetate anion (Erlenmeyer–Plöchl synthesis, Fig. 7). Details of the experimental procedure can be found elsewhere.[11,17] The purity of the compounds was monitored by the IR and the NMR spectroscopy. The melting points found are listed in Table 5. The UV-VIS absorption bands in the 70% (v/v) aqueous dioxane were not single peaks but had a vibrational structure. The peak maxima are presented in Table 5.

Table 5 Melting points of the compounds, recrystallization solvents and wavelengths (in nm) of the peak maximum in 70% aqueous dioxane for compounds **1** and **2**.

Cmpd.	m.p./°C	Recrystal. Solvent	λ_{max}
1a	147–150	Ethanol	377
1b	140–143	Ethanol	378
1c	141–143	Ethanol	379
2a	124–127	Ethanol	377
2b	129–132	Ethanol	379
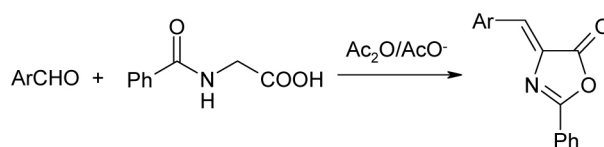
Fig. 7: Erlenmeyer–Plöchl synthesis.

The IR spectra were recorded for the chlorophorm solutions of the compounds **1** and **2** on a Zeiss Specord M-80 spectrometer at room temperature using NaCl cells of 0.1 cm thickness. The concentration of the compounds was 12.0×10^{-3} mol dm^{-3}. The CHCl$_3$ was of spectroscopic purity (Merck). The peak positions were referenced to the standard spectrum of polystyrene.

The ^1H and ^{13}C NMR spectra of the **1a–c**, **2a,b** were recorded for saturated CDCl$_3$ solutions at 300 K with a Bruker Avance DPX spectrometer working at 200.13 MHz for proton and 50.32 MHz for ^{13}C, respectively. The chemical shifts were referenced to the signal of TMS. The individual chemical shifts (in ppm) and results of elemen-

tal analyses (performed with a Perkin Elmer 2400 elemental analyzer) for the compounds **1a–c**, **2a,b** are given below.

(4Z)-2-(4-Butoxyphenyl)-4-(3-nitrobenzylidne)-1,3-oxazol-5(4H)-one (1a): ^{1}H NMR δ 1.10 (t, 3H, CH_3CH$_2$CH$_2$CH$_2$O); 1.75 (sx, 2H, CH$_3$CH_2CH$_2$CH$_2$O); 1.96 (p, 2H, CH$_3$CH$_2$CH_2CH$_2$O); 4.24 (t, 2H, CH$_3$CH$_2$CH$_2$CH_2O); 7.06–7.41 (m, 3H); 7.78 (t, 1H, Ar-*H*); 8.20–8.55 (m, 4H, Ar-*H*); 9.35 (s, 1H, Ar-*H*). ^{13}C NMR δ 14.18, 19.53, 31.39, 68.41, 115.15, 116.81, 124.53, 125.77, 126.29, 129.68, 130.87, 135.28, 135.88, 137.21, 148.50, 164.06, 164.81, 166.89. Anal. Calcd for C$_{20}$H$_{18}$N$_2$O$_5$: C, 65.57; H, 4.95; N, 7.65. Found: C, 65.88; H, 4.61; N, 7.52.

4-[(Z)-(2-(4-Butoxyphenyl)-5-oxo-1,3-oxazol-4(5H)-ylidene)methyl]phenyl 4-methylbenzenesulfonate (1b): ^{1}H NMR δ 1.17 (t, 3H, CH_3CH$_2$CH$_2$CH$_2$O); 1.70 (m, 2H, CH$_3$CH_2CH$_2$CH$_2$O); 1.98 (m, 2H, CH$_3$CH$_2$CH_2CH$_2$O); 2.62 (s, 3H, CH_3-Ar); 4.21 (t, 2H, CH$_3$CH$_2$CH$_2$CH_2O); 7.12–7.25 (m, 5H); 7.48 (d, 2H, Ar-*H*); 7.88 (d, 2H, Ar-*H*); 8.16–8.30 (m, 4H, Ar-*H*). ^{13}C NMR δ 14.17, 19.51, 22.06, 31.38, 68.32, 115.02, 117.19, 122.77, 127.79, 128.50, 129.90, 130.51, 132.20, 132.67, 133.46, 134.07, 145.61, 150.78, 163.67, 163.84, 167.43. Anal. Calcd for C$_{27}$H$_{25}$NO$_6$S: C, 65.97; H, 5.13; N, 2.85. Found: C, 66.53; H, 5.01; N, 2.84.

(4Z)-2-(4-Butoxyphenyl)-4-(4-chlorobenzylidene)-1,3-oxazol-5(4H)-one (1c): ^{1}H NMR δ 1.00 (t, 3H, CH_3CH$_2$CH$_2$CH$_2$O); 1.54 (sx, 2H, CH$_3$CH_2CH$_2$CH$_2$O); 1.81 (p, 2H, CH$_3$CH$_2$CH_2CH$_2$O); 4.04 (t, 2H, CH$_3$CH$_2$CH$_2$CH_2O); 6.95–7.05 (m, 3H); 7.38–7.43 (d, 2H, Ar-*H*); 8.04–8.11 (m, 4H, Ar-*H*). ^{13}C NMR δ 14.00, 19.36, 31.27, 68.27, 102.09, 115.09, 117.44, 128.28, 129.26, 130.65, 132.43, 133.42, 134.09, 136.89, 163.84, 167.76. Anal. Calcd for C$_{20}$H$_{18}$ClNO$_3$: C, 67.51; H, 5.10; N, 3.94; Cl, 9.96. Found: C, 67.14; H, 5.08; N, 3.98; Cl, 9.61.

(4Z)-2-(4-Isobutoxyphenyl)-4-(3-nitrobenzylidene)-1,3-oxazol-5(4H)-one (2a): ^{1}H NMR δ 1.13 (d, 6H, (CH_3)$_2$CHCH$_2$O); 2.18 (m, 1H, (CH$_3$)$_2$CHCH$_2$O); 3.89 (d, 2H, (CH$_3$)$_2$CHCH_2O); 6.98–7.10 (m, 3H); 7.58–7.66 (m, 1H, Ar-*H*); 8.07 (m, 2H, Ar-*H*); 8.20 (dd, 1H, Ar-*H*); 8.35 (dd, 1H, Ar-*H*); 9.10 (s, 1H, Ar-*H*). ^{13}C NMR δ 19.50, 28.52, 74.90, 115.10, 116.73, 124.41, 125.62, 126.18, 129.59, 130.75, 135.19, 135.77, 137.10, 148.39, 164.05, 164.68, 166.69. Anal. Calcd for C$_{20}$H$_{18}$N$_2$O$_5$: C, 65.57; H, 4.95; N, 7.65. Found: C, 65.22; H, 5.00; N, 7.53.

4-[(Z)-(2-(4-Isobutoxyphenyl)-5-oxo-1,3-oxazol-4(5H)-ylidene)methyl!?πhenyl 4-methylbenzenesulfonate (2b): ^{1}H NMR δ 1.03 (d, 6H, (CH_3)$_2$CHCH$_2$O); 2.11 (m, 1H, (CH$_3$)$_2$CHCH$_2$O); 2.40 (s, 3H, CH_3-Ar); 3.80 (t,

2H, (CH$_3$)$_2$CHCH_2O); 6.88–7.05 (m, 5H); 7.26 (dd, 2H, Ar-*H*); 7.67 (d, 2H, Ar-*H*); 7.95–8.06 (m, 4H, Ar-*H*). ^{13}C NMR δ 19.51, 22.06, 28.52, 74.84, 115.00, 117.17, 122.71, 127.69, 128.44, 129.85, 130.45, 132.24, 132.62, 133.39, 134.03, 145.52, 150.73, 158.80, 163.75, 167.28. Anal. Calcd for C$_{27}$H$_{25}$NO$_6$S: C, 65.97; H, 5.13; N, 2.85. Found: C, 66.34; H, 5.31; N, 2.69.

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Povzetek

Članek predstavlja pet novih (4*Z*)-4-benziliden-2-fenil-1,3-oksazol-5(4*H*)-onov (azlaktonov), raziskanih s pomočjo infrardeče (IR) ter jedrske magnetne resonančne spektroskopije (NMR) jeder ^{1}H in ^{13}C. Spektroskopske lastnosti oksazolskega obroča smo spremljali glede na substituente na benzilidenskem oz. fenilnem obroču. Spojine smo pripravili z Erlenmeyer–Plöchlov sintezo iz ustrezno substituiranih aldehidov in hipurne kisline. IR absorpcijski spektri, izmerjeni v kloroformu, so pokazali jasen razcep vibracijskih trakov v območju, ki je značilno za karbonilne raztezne (*stretching*) vibracije. Ta razcep se lahko pripiše Fermijevi resonanci; izračunali smo tudi valovna števila karbonilnih stretching trakov v neperturbiranih sistemih. Asignirali smo tudi kemijske premike ogljikov oksazolonskega obroča. Vpliv substituentov na spektralne lastnosti je bil raziskan in razložen. Ugotovljeno je bilo tudi, da oksazolonska molekula vsebuje razpotegnjen π-elektronski sistem, po katerem se elektronski vplivi učinkovito prenašajo.