

Contents lists available at ScienceDirect

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy



journal homepage: www.elsevier.com/locate/saa

Vibrational spectra of phenyl acridine-9-carboxylates and their 10-methylated cations: A theoretical and experimental study

B. Zadykowicz, A. Ożóg, K. Krzymiński*

Faculty of Chemistry, University of Gdańsk, J. Sobieskiego 18, 80-952 Gdańsk, Poland

ARTICLE INFO

ABSTRACT

Article history: Received 19 November 2009 Received in revised form 10 February 2010 Accepted 15 February 2010

Keywords:

Phenyl acridine-9-carboxylates 9-Phenoxycarbonyl-10-methylacridinium cations Vibrational spectra assignment Structural features Spectral versus physicochemical parameters relations Infrared spectra of phenyl acridine-9-carboxylates and their 10-methylated cationic derivatives were recorded and discussed. Experimental data were compared with theoretically predicted transitions at the DFT level of theory (using the B3LYP functional and 6-31G** basis set) for optimized geometries of molecules. Substitution influences the values of the wavenumbers of characteristic stretching and bend-ing modes, i.e. those corresponding to ester groups and fragments of molecules containing a heterocyclic nitrogen atom. The experimentally determined transitions of selected groups of atoms correlate well with the theoretically predicted values. Interdependences among some theoretically derived physicochemical features of the compounds and IR frequencies of selected bands are also discussed.

© 2010 Elsevier B.V. All rights reserved.

1. Introduction

Nitrogen substituted cationic derivatives of phenyl acridine-9carboxylates (acridinium esters) have long been of interest owing to their numerous applications in immunological assays [1–3] and chemical, biological, medical or environmental analyses [4–6]. These compounds are easily oxidized with hydrogen peroxide in alkaline media. Oxidation produces electronically excited 10-alkyl-9-acridinones and the process is accompanied by relatively efficient chemiluminescence in aqueous solutions (quantum yields of ca. 2%) [7–9]. In this context, 9-phenoxycarbonyl-10-methylacridinium cations and their precursors–phenyl acridine-9-carboxylates [10–12,13] and the 9-cyano-10-methylacridinium cation were recently investigated [14].

Vibrational spectroscopy is a useful tool for acquiring a better understanding of the structure and molecular properties of organic compounds [15,16]. It is an important method for studying small molecules as well as biological systems, i.e. the constituents of nucleic acids, DNA and RNA [17]. FT-IR spectroscopy is particularly useful, especially when coupled with theoretical methods. It is a convenient means of obtaining theoretical estimates of the position of bands arising from given molecular oscillations so that they can be recognized in experimental spectra. Computational methods are increasingly applied to compounds with the aim of elucidating their structures, electronic properties, mechanism of formation and other properties [8,18].

In this paper we present the results of IR spectroscopy investigations of selected phenyl acridine-9-carboxylates and their 10-methylated salts (Scheme 1, Table 1) that we think are interesting for the above-mentioned reasons. It is known that the chemiluminescence parameters of the latter, like decay constants and emission efficiency, are affected to a greater or lesser extent when the structure of the aromatic ester fragment is altered [19]. In order to find out whether this does actually happen, investigations were undertaken on phenyl 10-methylacridinium-9-carboxylates. which contain substituents in the benzene ring differing in their electronic and steric effects [13]. This unique set of experimental and theoretical data also provided an opportunity to observe how the structures of 9-phenoxycarbonyl-10-methylacridinium cations and phenyl acridine-9-carboxylates affect their infrared spectra, and how band positions are related to the structural and physicochemical characteristics of this important group of chemiluminogenic compounds.

2. Methods

2.1. Experimental

Compounds **1a–1d** (Scheme 1, Table 1) were synthesized as described previously [12,20,21]. Briefly, 9-(chlorocarbonyl)acridine was esterified at room temperature with the appropriate hydroxybenzene (phenol, 2-fluorophenol, 2-methoxyphenol,

^{*} Corresponding author. Tel.: +48 58 523 54 67; fax: +48 58 345 04 64. *E-mail address*: karolk@chem.univ.gda.pl (K. Krzymiński).

^{1386-1425/\$ –} see front matter $\ensuremath{\mathbb{C}}$ 2010 Elsevier B.V. All rights reserved. doi:10.1016/j.saa.2010.02.014



Scheme 1. Canonical structures of phenyl acridine-9-carboxylates (1) and 9-phenoxycarbonyl-10-methylacridinium cations (2) (Table 1).

2-nitrophenol) in anhydrous dichloromethane in the presence of *N*,*N*-diethylethanamine and *N*,*N*-dimethyl-4-pyridinamine. The crude products, chromatographically purified on SiO₂ (cyclohexane/ethyl acetate, 3:2 v/v), gave yields in the range of 60–80%. The esters obtained were subjected to elemental analyses (EAGER 200, Carlo Erba Instruments) and TLC tests in the above-mentioned system. The % of elements found/calculated, retention factors (R_f) and melting points (m.p., in K) were as follows (**1a**): C 79.79/80.25, H 4.44/4.38, N 4.25/4.68, R_f =0.38, m.p.=463–465; (**1b**): C 75.46/75.70, H 3.98/3.81, N 4.26/4.41, R_f =0.59, m.p.=436–437; (**1c**): C 76.45/76.58, H 4.55/4.59, N 4.22/4.25, R_f =0.56, m.p.=460–462; (**1d**): C 69.71/69.76, H 3.46/3.51, N 8.10/8.14, R_f =0.52, m.p.=421–422.

The phenyl acridine-9-carboxylates were quaternalized using excess of methyl trifluoromethanesulphonate dissolved an dichloromethane at room temperature. 10-Methyl-9in (phenoxycarbonyl)-acridinium salts 2a-2d (Scheme 1, Table 1) were purified using repeated precipitation with an excess of ethyl ether from ethanolic solution and subjected to elemental analysis and HPLC chromatography (Waters 600 E Multisolvent Delivery System, Waters 2487 Dual λ Absorbance Detector; mobile phase: acetonitrile/0.1 M TFA = 1/1.5 (40%/60%); stationary phase: C-8 column, 3×150 mm, 'Symmetry'). Elemental analyses (% of elements found/calculated), retention times (R_t , in minutes) and melting points (m.p., in K) were as follows (2a): C 56.27/57.02, H 3.42/3.48, N 2.72/3.02, $R_t = 0.38, m.p. = 500 - 502;$ (**2b**): C 55.73/54.89, H 3.23/3.14, 2.82/2.91, $R_t = 3.72$, m.p. = 501–503; (2c): C 52.94/51.97, Ν H 3.16/2.97, N 5.36/5.51, $R_t = 3.79$, m.p. = 514–516; (2d): C 51.63/51.98, H 2.92/2.85, N 2.64/2.64, R_t = 4.20, m.p. = 506–508. Structural, NMR and mass spectrometry data for the compounds presented here will be discussed in a separate paper. The crystal structure of compound **2d** was determined by the X-ray method [11].

The FT-IR spectra of all compounds were recorded at room temperature in the 5000–400 cm⁻¹ range (resolution ± 4 cm⁻¹) using a Bruker IFS 66 FTIR spectrometer and the KBr pellet technique.

2.2. Theoretical

Unconstrained geometry optimizations of isolated molecules were carried out at the density functional level of theory (DFT) [22] using the gradient technique [23], the 6–31G** basis set [24,25] and the Becke 3LYP (B3LYP) non-local spin density exchange functional [26,27]) supplemented with the Lee–Yang–Parr non-local correlation functional [28]. After completion of each optimization, the Hessian (second derivatives of the energy as a function of nuclear coordinates) was calculated and checked for positive definiteness in order to assess whether the structures were true minima [29]. The harmonic vibrational frequencies (wave numbers) were subsequently derived from the numerical values of these second derivatives. These wavenumbers were then scaled by multiplying them by 0.96 [30].

The calculations were carried out on computers of the Tri-City Academic Network Computer Centre in Gdansk (TASK) using the GAUSSIAN 03 program package [31]. Structural data and dipole moments were extracted directly from files following the geometry optimizations. The atomic partial charges were those reproduc-

Table 1	
The compounds investigated (Scheme 1)	١

	·						
Compound no.	Compound name*	R					
Phenyl acridine-9-carboxylates (1)							
1a	Phenyl acridine-9-carboxylate	Н					
1b	2-Fluorophenyl acridine-9-carboxylate	F					
1c	2-Methoxyphenyl acridine-9-carboxylate	OCH ₃					
1d	2-Nitrophenyl acridine-9-carboxylate	NO_2					
9-Phenoxycarbonyl-10-methylacridinium cations (2)							
2a	9-Phenoxycarbonyl-10-methylacridinium	Н					
2b	9-(2-Fluorophenoxy)carbonyl-10-methylacridinium	F					
2c	9-(2-Methoxyphenoxy)carbonyl-10-methylacridinium	OCH ₃					
2d	9-(2-Nitrophenoxy)carbonyl-10-methylacridinium	NO_2					

* For **1**, the compound is named; for **2**, the cation is named.



Fig. 1. DFT-optimized geometries of the entities shown in Scheme 1.

ing molecular electrostatic potential around molecules (MEP fitted charges) [32].

3. Results and discussion

As our recent X-ray investigations showed, the acridine nucleus in phenyl acridine-9-carboxylates containing an alkyl group in the benzene ring is practically flat, being distorted from planarity by less than 2° [10,33,34]. The C₍₉₎C₍₁₅₎ bond lengths are typical, reaching values of about 1.49 Å. The recently published crystal structure of **2d** shows that distortion from planarity is negligible in this cation, with values of <2° [11]. The acridine ring in the cation is somewhat twisted along the C₍₉₎N₍₁₀₎ axis, as suggested by the different dihedral angles within the central ring. The C₍₉₎C₍₁₅₎ and N₍₁₀₎C₍₂₄₎ bond lengths have respective values of about 1.51 Å and 1.47 Å. The carboxyl group is twisted at an angle of 65.8° or 67.0° relative to the acridine skeleton, while the acridine and benzene ring systems in the cation are respectively oriented at 3.0° or 11.1° to each other.

The structures of compounds **1a–1d** and **2a–2d** obtained from DFT optimizations are shown in Fig. 1. According to the theoretical predictions, their structural features depend only minimally on the type of substituents present in the phenoxycarbonyl fragment (Table 2); differences are more pronounced if uncharged and charged derivatives are compared. The acridine skeleton is almost planar in **1a–1d**, as values between -0.6° and -1.4° were obtained for the dihedral angle $C_{(12)}N_{(10)}C_{(13)}C_{(14)}$ and between 0.5° and -0.2° for the dihedral angle $C_{(11)}C_{(9)}C_{(14)}C_{(13)}$. In contrast,

the central ring in **2a**–**2d** is more or less convex at the nitrogen atom site and concave at the ester group site, as the values of the above dihedral angles lie between -8.6 and -8.9° and $7.4 - 7.9^{\circ}$ respectively; values are highest for the 2-nitro cation (**2d**). Similar conclusions can be drawn from an analysis of the values of the $C_{(12)}C_{(11)}C_{(9)}C_{(14)}/C_{(11)}C_{(9)}C_{(14)}C_{(13)}$ dihedral angles. The $C_{(9)}C_{(15)}$ bond lengths in the uncharged derivatives

The $C_{(9)}C_{(15)}$ bond lengths in the uncharged derivatives (**1a-1d**) are almost identical, having values of around 1.50 Å. The analogous lengths for **2a-2d** are comparable–ca 1.51 Å. The $N_{(10)}C_{(12)}/N_{(10)}C_{(13)}$ bond lengths are almost the same for a given entity. They are somewhat greater in cations but generally typical of aromatic heterocyclic systems. The length of the $N_{(10)}C_{(24)}$ bond is practically constant in all of the cations, having a value of around 1.48 Å.

The carboxyl group is twisted at angles from 51.3° (for **1a**) to 55.9° (for **2d**) relative to the acridine skeleton. The acridine and benzene ring systems are oriented at about $54^{\circ}-86^{\circ}$ in **1a–1d** and $48^{\circ}-83^{\circ}$ in cations **2a–2d**. No relationships were found between the substituents' size parameters (Charton's size values or Taft size parameters [35]) and the theoretically established orientation of the benzene ring in both series of acridine derivatives.

The dipole moments, calculated for the uncharged esters (**1a-1d**), are also presented in Table 2. As expected, the 2-nitro derivative (**1d**) has the largest dipole moment, and the unsubstituted ester **1a** the lowest.

To the best of our knowledge, no systematic experimental or quantum mechanical vibrational data have been reported for phenyl acridine-9-carboxylates and their 10-methylated derivatives. However, spectral data, including infrared spectra have been

Table 2

Theoretically p	predicted structural and	physicochemical of	characteristics of pher	vl acridine-9-carbox	vlates and their cationic deriv	atives.
				J	J	

Compound	Bond length (Å)			Angle (°)		Dipole moment (D)	LCAO co p _z LUMC	efficient of tl) orbital at	ne MEP fitted	charge
	C(9)C(15)	$N_{(10)}C_{(12)}/N_{(10)}C_{(13)}$	A ^a	B ^a	C ^a		C ₍₉₎	C(15)	C ₍₉₎	C ₍₁₅₎
1a	1.501	1.341/1.341	-0.1/-1.1	-1.8/0.8	85.5	1.99	0.291	0.0832	-0.163	0.734
1b	1.498	1.341/1.341	0.5/-1.4	-2.5/1.8	54.4	2.76	0.286	0.0726	-0.150	0.730
1c	1.502	1.341/1.341	-0.2/-0.8	-1.1/0.2	54.8	3.09	0.280	0.0501	-0.0650	0.655
1d	1.496	1.341/1.341	-0.2/-0.6	-0.9/0.2	75.1	4.58	0.256	0.0680	-0.151	0.748
2a	1.515	1.379/1.379	7.4/-8.6	-4.7/3.6	83.0		0.314	0.0256	-0.201	0.695
2b	1.513	1.379/1.379	7.9/-8.7	-5.2/4.4	48.0		0.177	0.0249	-0.218	0.699
2c	1.514	1.379/1.378	7.6/-8.8	-4.7/3.5	48.4		0.293	0.0263	-0.221	0.682
2d	1.515	1.378/1.378	7.9/-8.9	-4.7/3.7	66.3		0.299	0.0473	-0.163	0.719

^a A, dihedral angle $C_{(11)}C_{(12)}N_{(10)}C_{(13)}/C_{(12)}N_{(10)}C_{(13)}/C_{(14)}$; B, dihedral angle $C_{(12)}C_{(11)}C_{(9)}C_{(14)}/C_{(11)}C_{(9)}C_{(14)}C_{(13)}$; C, dihedral angle between the mean plane of the acridine nucleus and the mean plane of the benzene ring.

Table 3

Selected vibrational transitions in phenyl acridine-9-carboxylates and their cationic derivatives.

Compound no.	Mode			Wavenumber (cm ⁻¹)		
	No.	Туре	Description	Experimental	Theoretical	
1a	V89	ν _I	C=O stretching	1748	1777	
	V73	$\nu_{\rm II}$	Molecular deformation involving N(10)	1352	1346	
	v_{66}	$v_{\rm III}$	$C_{(15)}-O_{(17)}-C_{(18)}$ in plane bending	1196	1203	
	v_{37}	$\nu_{\rm IV}$	Out of plane C–H bending	752	777	
1b	V90	$\nu_{\rm I}$	C=O stretching	1757	1795	
	v_{74}	$\nu_{\rm II}$	Molecular deformation involving N(10)	1350	1348	
	ν_{61}	ν_{III}	$C_{(15)}-O_{(17)}-C_{(18)}$ in plane bending	1142	1139	
	v_{37}	$\nu_{\rm IV}$	Out of plane C–H bending	753	754	
1c	v_{99}	$\nu_{\rm I}$	C=O stretching	1751	1792	
	v_{80}	$v_{\rm II}$	Molecular deformation involving N(10)	1352	1348	
	v_{68}	$v_{\rm III}$	$C_{(15)}-O_{(17)}-C_{(18)}$ in plane bending	1158	1162	
	V42	$\nu_{\rm IV}$	Out of plane C–H bending	746	772	
1d	v_{96}	$\nu_{\rm I}$	C=O stretching	1754	1797	
	V91		NO2 bending (asymmetrical) + molecular deformation	1591	1592	
	v_{80}	$v_{\rm H}$	Molecular deformation involving N(10)	1347	1373	
	v_{65}	$v_{\rm III}$	$C_{(15)}-O_{(17)}-C_{(18)}$ in plane bending	1133	1130	
	v_{41}	$\nu_{\rm IV}$	Out of plane C–H bending	766	769	
2a	V98	$\nu_{\rm I}$	C=O stretching	1762	1783	
	v_{80}	$v_{\rm II}$	Molecular deformation involving N(10)	1376	1371	
	v_{72}	$v_{\rm III}$	$C_{(15)}-O_{(17)}-C_{(18)}$ in plane bending	1211	1224	
	v_{38}	$\nu_{\rm IV}$	Out of plane C–H bending	752	753	
2b	V99	$\nu_{\rm I}$	C=O stretching	1762	1804	
	ν_{81}	$v_{\rm II}$	Molecular deformation involving N(10)	1377	1372	
	V72	$v_{\rm III}$	$C_{(15)}-O_{(17)}-C_{(18)}$ in plane bending	1203	1208	
	v_{41}	$\nu_{\rm IV}$	Out of plane C–H bending	767	762	
2c	v_{107}	$\nu_{\rm I}$	C=O stretching	1762	1787	
	v_{86}	v_{II}	Molecular deformation involving N(10)	1376	1370	
	V77	$v_{\rm III}$	$C_{(15)} - O_{(17)} - C_{(18)}$ in plane bending	1206	1214	
	V43	$\nu_{\rm IV}$	Out of plane C–H bending	754	758	
2d	v_{105}	$\nu_{\rm I}$	C=O stretching	1764	1802	
	V99		NO2 bending (asymmetrical) + molecular deformation	1582	1585	
	v_{86}	$\nu_{\rm II}$	Molecular deformation involving N(10)	1375	1376	
	V77	$v_{\rm III}$	$C_{(15)} - O_{(17)} - C_{(18)}$ in plane bending	1197	1206	
	V ₄₄	$\nu_{\rm IV}$	Out of plane C–H bending	768	762	

presented as structural proof for some acridinium esters employed as chemiluminogenic tracers [36,37]. The detailed vibrational assignments of selected modes of phenyl acridine-9-carboxylates and their 10-methylated cationic derivatives (Scheme 1), along with the calculated normal mode descriptions, are reported in Table 3. Infrared spectra of selected compounds (1d, 2d), together with the theoretically determined vibrational wavenumbers are illustrated in Fig. 2. Thorough analysis of the spectra of all the compounds revealed that they reflect features of both acridinium ester moiety and substituents. The transitions relating to the substituents are unique to a given compound. On the other hand, the transitions relating to the acridine ester fragment display numerous similarities. In the latter case, band positions differed only insignificantly from compound to compound, being related to some extent to the structural and physicochemical properties of the molecules under investigation.

We compared the calculated wavenumbers for phenyl acridine-9-carboxylates and their cationic forms methylated at the endocyclic N atom with the experimental values. When analysing the spectra with the aid of 'animations' of molecular vibrations, we selected four of them that were characteristic of all the compounds investigated. These are the C=O stretching vibration (v_I), the molecular deformation involving N₍₁₀₎ (v_{II}), the C₍₁₅₎-O₍₁₇₎-C₍₁₈₎ in plane bending vibration (v_{III}) and the out of plane C–H bending vibration (v_{IV}). All the experimental and predicted characteristic transitions and the specific vibrations relating to the presence of substituents are given in Table 3. The theoretically predicted transitions for isolated molecules sometimes corresponded to the experimentally determined characteristics, but in most cases they differed from them by $<43 \text{ cm}^{-1}$. The differences between the experimental and theoretical values were relatively large in the case of the C=O stretching vibrations.

Fig. 3 illustrates the relationships between the calculated and experimental wavenumbers for **1a** and **2a**. Both correlations are linear and are characterized by high correlation coefficients. These relationships confirm that the computational results correspond well to the experimental ones. These types of correlations were investigated for the other derivatives, and in all cases the linear correlation coefficients were 0.99 or higher.

We also examined the relationships between selected experimental frequencies (Table 3) and tabularized constants characterizing the electronic or steric properties of substituents [38]. The most pronounced correlation (Fig. 4) was found between the frequency of $C_{(15)}-O_{(17)}-C_{(18)}$ in plane bending (ν_{III}) and the inductive sigma constant (σ_1) of the substituents (H, F, OCH₃, NO₂) [35]. Generally, the frequency of this vibration is inversely proportional to the rise in value of σ_1 in the series of compounds **2a–2d**. Interestingly, the correlation for phenyl acridine-9-carboxylates (**1a–1d**) is multinomial. From the data in Fig. 4 it emerges that the energy of the $C_{(15)}-O_{(17)}-C_{(18)}$ vibrations falls in the order: **1a > 1c > 1b > 1d** and **2a > 2c > 2b > 2d**. The $C_{(15)}-O_{(17)}-C_{(18)}$ frequencies characteristic of cations are generally higher than for those of esters and seem to be less sensitive to changes in the polarity of the substituent in the ester fragment.



Fig. 2. FT-IR spectra of 2-nitrophenyl acridine-9-carboxylate (**1d**; A); calculated FT-IR spectra of **1d** (B); 9-(2-nitrophenoxy)carbonyl-10-methylacridinium (**2d**; C); calculated FT-IR spectrum of **2d** (D).

In the case of compounds **2a–2d** we also noted a trend between the frequency of the v_{I} , v_{III} vibrations (Table 3) and the MEP fitted atomic partial charge at $C_{(9)}$ (Table 2). These relationships, presented in Fig. 5, are linear. The MEP fitted atomic partial charge may be one of the parameters related to the chemiluminogenic properties of acridinium esters, as $C_{(9)}$ is the site of the primary nucleophilic attack of OOH- in the step initiating the 'light path of reaction' [7,8]. However, it must be noted that the values of the MEP fitted charge at $C_{(9)}$ are lower than the ones characterizing $C_{(15)}$. On the other hand, molecular centres sensitive to nucleophilic attack are also determined by LUMO distribution in an electrophilic species (cations), as indicated by the Frontier Orbital Theory [38]. The values of the LCAO coefficients of the p_z atomic orbital in **2a**-**2d** LUMO are ca 6–12 times higher at the endocyclic $C_{(9)}$ than at the carbonyl group carbon atom (Table 2). This implies that $C_{(9)}$ rather than the carbon atom of the carbonyl group is the site of the primary nucleophilic attack of the above-mentioned anions. On the other hand, the trends of both MEP fitted charges and LCAO coefficients of the p_z atomic orbital indicate that **2a** and **2d** should be



Fig. 4. Relationships between wavenumbers of $C_{(15)}$ – $O_{(17)}$ – $C_{(18)}$ in plane bending vibration (ν_{III} , Table 3) and the inductive sigma constant (σ_1) of the substituents.



MEP fitted charge at $C_{(15)} = 0.0163v_1 - 27.958$ (correlation coefficient, 0.863)

Fig. 5. C=O stretching wavenumbers for **2a-2d** (ν_I , Table 3) versus MEP fitted charges at the C₍₉₎ and C₍₁₅₎ atoms (Table 2).

the most susceptible to nucleophilic attack at $C_{(9)}$; this has been confirmed experimentally.

4. Concluding remarks

In summary, four new phenyl acridine-9-carboxylates and their 10-methylated cationic derivatives were synthesized, examined in terms of their purity and structure, and subjected to advanced infrared spectroscopic investigations. The experimental results were compared with the theoretical ones obtained at the level of density functional theory. Comparison of the experimental and calculated vibrational frequencies indicates that the B3LYP results are



Fig. 3. Correlation between the calculated and experimental wavenumbers for phenyl acridine-9-carboxylate (**1a**, left) and the 9-phenoxycarbonyl-10-methylacridinium cation (**2a**, right) (the data represent transitions in the 490–1700 cm⁻¹ range). The equations are: $v_{\text{theor.}} = 0.989 v_{\text{exp.}} + 19.51$ (correlation coefficient, 0.996) (**1a**) and $v_{\text{theor.}} = 1.008 v_{\text{exp.}} + 2.72$ (**2a**) (correlation coefficient, 0.998).

in reasonable agreement with the experimental ones. Additionally, the DFT structures and structural parameters found in the work are generally in good agreement with the crystallographic data reported earlier.

The correlations found between the experimental values of wavenumbers of selected bands and the inductive constants of substituents, as well as the MEP fitted charges at the $C_{(9)}$ atom reveal the existence of structural-physicochemical property trends in this group of compounds. These findings provide a good starting tool for the search for new acridinium esters with practical applications as chemiluminogenic tracers.

Acknowledgements

This study was financed from the State Funds for Scientific Research though Grant No. N204 123 32/3143 (contract No. 3143/H03/2007/32) of the Polish Ministry of Research and Higher Education, for the period 2007–2010.

References

- L. Weeks, L. Beheshti, F. McCapra, A.K. Campbell, J.S. Woodhead, Clin. Chem. 29 (1983) 1474.
- [2] R. Hart, L. Taaffe, J. Immunol. Meth. 101 (1987) 91.
- [3] G. Zomer, J.F.C. Stavenuiter, R.H. van den Berg, E.H.J.M. Jansen, in: W.R.G. Baeyens, D. De Keukeleire, K. Korkidis (Eds.), Practical Spectroscopy Series, vol. 12, Marcel Dekker, New York, 1991, p. 505.
- [4] I.M. Warner, S.A. Soper, L.B. McGown, Anal. Chem. 68 (1996) 73.
- [5] C. Dodeigne, L. Thunus, R. Lejeune, Talanta 51 (2000) 415.
- [6] G. Zomer, M. Jacquemijns, in: A.M. Garcia-Campana, W.R.G. Baeyens (Eds.), Chemiluminescence in Analytical Chemistry, Marcel Decker, New York, 2001, p. 529.
- [7] F. McCapra, in: R.M. Acheson (Ed.), Chemistry of Heterocyclic Compounds, vol. 9, John Wiley and Sons, Inc, 1973, p. 615.
- [8] J. Rak, P. Skurski, J. Błażejowski, J. Org. Chem. 64 (1999) 3002.
- [9] A. Roda, M. Guardigli, E. Michelini, M. Mirasoli, P. Pasini, Anal. Chem. A75 (2003) 462.
- [10] A. Sikorski, K. Krzymiński, A. Konitz, J. Błażejowski, Acta Crystallogr. C61 (2005) o50.
- [11] A. Sikorski, K. Krzymiński, A. Niziołek, T. Lis, J. Błażejowski, Acta Crystallogr. E64 (2008) 0372.
- [12] K. Krzymiński, A.D. Roshal, A. Niziołek, Spectrochim. Acta A 70 (2008) 394.
- [13] K. Krzymiński, A. Niziołek, A.D. Roshal, A. Wróblewska, P. Malecha, J. Błażejowski, J. Org. Chem., submitted for publication.

- [14] A. Wróblewska, O.M. Huta, S.V. Midyanyj, I.O. Patsay, J. Rak, J. Błażejowski, J. Org. Chem. 69 (2004) 1607.
- [15] L. Rivas, A. Murza, S. Sánchez-Cortés, J.V. García-Ramos, Vib. Spectrosc. 25 (2001) 19.
- [16] S. Cîntã Pînzaru, C. Morari, Spectrochim. Acta A 60 (2004) 337.
- [17] S. Woutersen, P. Hamm, J. Chem. Phys. 115 (2001) 7737.
- [18] Y. Ebead, A.D. Roshal, A. Wróblewska, A.O. Doroshenko, J. Błażejowski, Spectrochim. Acta A 66 (2007) 1016.
- [19] G. Zomer, J.F.C. Stavenuiter, Anal. Chim. Acta 227 (1989) 11.
- [20] N. Sato, Tetrahedron Lett. 37 (1996) 8519.
- [21] A. Sikorski, K. Krzymiński, A. Niziołek, J. Błażejowski, Acta Crystallogr. C61 (2007) o690.
- [22] J.K. Labanowski, J.W. Anzelm, Density Functional Methods in Chemistry, Springer, New York, 1991.
- [23] H.B. Schlegel, Modern Electronic Structure Theory: Geometry Optimization on Potential Energy Surface, World Scientific, Singapore, 1994.
- [24] M.M. Francl, W.J. Pietro, W.J. Hehre, J.S. Binkley, M.S. Gordon, D.J. DeFrees, J.A. Pople, J. Chem. Phys. 77 (1982) 3654.
- [25] P.C. Hariharan, J.A. Pople, Theor. Chim. Acta 28 (1973) 213.
- [26] A.D. Becke, Phys. Rev. A 38 (1988) 3098.
- [27] A.D. Becke, J. Chem. Phys. 98 (1993) 1372, 5648.
- [28] C. Lee, W. Yang, R.G. Parr, Phys. Rev. B 37 (1988) 785.
- [29] N.C. Handy, D.J. Tozer, G.J. Laming, C.W. Murray, R.D. Amos, Isr. J. Chem. 33 (1993) 331.
- [30] J. Rak, P. Skurski, M. Gutowski, L. Jóźwiak, J. Błażejowski, J. Phys. Chem. A 101 (1997) 283.
- [31] M.J. Frish, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, J.A. Montgomery, T. Vreven, K.N. Kudin, J.C. Burant, J.M. Millam, S.S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G.A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J.E. Knox, H.P. Hratchian, J.B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, P.Y. Ayala, K. Morokuma, G.A. Voth, P. Salvador, J.J. Dannenberg, V.G. Zakrzewski, S. Dapprich, A.D. Daniels, M.C. Strain, O. Farkas, D.K. Malick, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J.V. Ortiz, Q. Cui, A.G. Baboul, S. Clifford, J. Cioslowski, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R.L. Martin, D.J. Fox, T. Keith, M.A. Al-Laham, C.Y. Peng, A. Nanayakkara, M. Challacombe, P.M.W. Gill, B. Johnson, W. Chen, M.W. Wong, C. Gonzalez, J.A. Pople, GAUSSIAN 03, Revision C.02, Gaussian, Inc., Wallingford, CT, 2004.
- [32] B.H. Besler, K.M. Merz, P.A. Kollman, J. Comput. Chem. 11 (1990) 431.
- [33] J. Meszko, K. Krzymiński, A. Konitz, J. Błażejowski, Acta Crystallogr. C58 (2002) 0157.
- [34] A. Sikorski, K. Krzymiński, A. Białońska, T. Lis, J. Błażejowski, Acta Crystallogr. E62 (2006) 0555.
- [35] C. Hansch, A. Leo, Substituent Constants for Correlation Analysis in Chemistry and Biology, Wiley Interscience, New York, 1979.
- [36] K. Smith, Z. Li, J.-J. Yang, I. Weeks, J.S. Woodhead, J. Photochem. Photobiol. A: Chem. 132 (2000) 181.
- [37] Z. Razavi, F. McCapra, Luminescence 15 (2000) 239.
- [38] I. Fleming, Frontier Orbitals and Organic Chemical Reactions, Wiley, London, New York, 1976.