



Procesing '20

Zbornik radova

**Beograd
10. septembar 2020**

ZBORNIK RADOVA Proceedings

**pisanih za 33. Međunarodni kongres
o procesnoj industriji**



2020

ZBORNİK RADOVA
pisanih za 33. Međunarodni kongres
o procesnoj industriji
Hotel „Zepter“, Beograd
10. septembar 2020.

Izdavač
Savez mašinskih i elektrotehničkih
inženjera i tehničara Srbije (SMEITS)
Društvo za procesnu tehniku
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Tiraž
150 primeraka

CD umnožava
Paragon, Beograd

ISBN
978-86-85535-05-5

CIP - Каталогизација у публикацији
Народна библиотека Србије, Београд

621(082)(0.034.2)
66.01(082)(0.034.2)

МЕЂУНАРОДНИ конгрес о процесној индустрији ПРОЦЕСИНГ (33 ; 2020 ; Београд)

Zbornik radova [pisanih za 33. Međunarodni kongres o procesnoj industriji], PROCESING '20, Beograd, 10. septembar 2020. [Elektronski izvor] / [organizatori Društvo za procesnu tehniku pri SMEITS-u [i] Katedra za procesnu tehniku Mašinskog fakulteta u Beogradu] ; [urednici Miroslav Stanojević, Aleksandar Jovović]. - Beograd : Savez mašinskih i elektrotehničkih inženjera i tehničara Srbije (SMEITS), Društvo za procesnu tehniku, 2020 (Beograd : Paragon). - 1 elektronski optički disk (CD-ROM) ; 12 cm

Sistemska zahtevi: Nisu navedeni. - Radovi na srp. i engl. jeziku. - Nasl. sa naslovne strane dokumenta. - Tiraž 150. - Bibliografija uz svaki rad. - Abstracts.

ISBN 978-86-85535-05-5

a) Mašinstvo -- Зборници б) Процесна индустрија -- Зборници

COBISS.SR-ID 25087497

Organizatori



Društvo za procesnu tehniku
pri SMEITS-u



Katedra za procesnu tehniku
Mašinskog fakulteta u Beogradu

Održavanje 33. Procesinga finansijski je pomoglo
Ministarstvo prosvete, nauke i tehnološkog
razvoja Republike Srbije



Programski pokrovitelji

- TEHNOLOŠKO-METALURŠKI FAKULTET UNIVERZITETA U BEOGRADU
- FAKULTET TEHNIČKIH NAUKA UNIVERZITETA U NOVOM SADU, NOVI SAD
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- MAŠINSKI FAKULTET UNIVERZITETA U NIŠU, NIŠ

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Wilo, Beograd
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PROUČAVANJE SOLVATOHROMNIH SVOJSTAVA NOVOG BENZILIDENHIDANTOINA KAO MOLEKULSKOG FOTOHROMNOG PREKIDAČA

SOLVATOCHROMIC STUDY OF NOVEL BENZYLIDENEHYDANTOIN AS A MOLECULAR PHOTOCHROMIC SWITCH

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Molekulski fotohromni prekidači predstavljaju male organske molekule ili supramolekulske vrste koji se mogu reverzibilno interkonvertovati između dva stabilna stanja pod dejstvom svetlosti. Nastala promena je najčešće posledica trans→cis fotoizomerizacije, fotociklizacije ili kombinacije ova dva procesa. U cilju kreiranja novih fotoaktivnih materijala, u ovom radu su prikazana dva različita načina sinteze (Z)-5-(4-dodeciloksi)benziliden)imidazolidin-2,4-diona, kao i kompletna strukturna karakterizacija ostvarena primenom različitih spektroskopskih metoda. U nastavku istraživanja, izvršena je solvatohromna analiza ovog jedinjenja snimanjem apsorpcionih spektara u odabranom setu rastvarača, a potom je razmatran uticaj specifičnih i nespecifičnih interakcija između molekula rastvarača i rastvorene supstance na položaj apsorpcionih maksimuma metodom linearne korelacije energije solvatacije, tj. Kamlet-Taftovom i Katalanovom jednačinom. Preliminarni rezultati ovog istraživanja dobra su polazna tačka za dizajniranje novih fotoaktivnih materijala sa širokim spektrom primene.

Ključne reči: molekulski prekidači; benzilidenhidantoini; solvatohromizam; fotoaktivni materijali.

Molecular photochromic switches represent an intriguing class of organic molecules that can be reversibly interconverted between two stable states by light. The resulting change may be the consequence of trans→cis photoisomerization, photocyclization or a combination of both. With the aim of development of novel light-sensitive materials, the present study reports two different ways of synthesis of (Z)-5-(4-dodecyloxy)benzylidene)imidazolidine-2,4-dione and its structural characterization by various spectroscopic techniques. Besides, the solvatochromic behavior of new benzylidenehydantoin derivative has been evaluated by recording the absorption spectra in the selected solvent set and evaluating effects of the specific and nonspecific solvent–solute interactions on the absorption maxima shifts using linear solvation energy relationship, i.e. equations proposed by Kamlet-Taft and Katalan. The preliminary results of this investigation represent promising starting point for design of novel photoactive materials with a broad spectrum of applications.

Key words: molecular switches; benzylidenehydantoin; solvatochromism; photoactive materials.

1 Introduction

Control of the features of compounds such as their magnetic, electrical and optical properties through an external trigger is very interesting design characteristic of new promising functional systems and smart materials. Useful aspects of light, namely clean, quick and remote operation without the need for direct contact to the material have encouraged the development of variety of photoswitching systems among the light-responsive materials as the most important [1]. Molecular photochromic switches denote an intriguing class of organic molecules that can be interconverted reversibly between two or more stable states by stimulus with light. The resulting change is a consequence of the

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molecular alteration produced by the *cis*→*trans* photoisomerization, photocyclization or a combination of the two. An ideal photochromic switch would display perfect photocontrol implying that irradiation at diverse wavelengths allows quantitative photoconversion between two forms. Attractive features of these systems involve their short responsive times, reversibility, clean and tunable input and ability to convert an optical input into a array of useful output signals. As such, the molecular switches perform a key role in biology and information technology and have developed into important components of advanced materials. This is illustrated by the fact that these compounds have already found commercial application in optical memory devices i.e. recordable compact discs, CD-R, light sensitive sunglasses and ophthalmological lenses. Also, there has been a growing interest in employing these materials as molecular electronics, smart surfaces, in control of supramolecular organization and nanomachinery [2]. A literature review indicated two main families of compounds recognition of molecular switches, those acting through the isomerization of a double bond such as azobenzenes and overcrowded alkenes and through a cyclization on process i.e. fulgides, diarylethenes, spiropyrane analogs and dihydroazulenes. The photoisomerization E→Z→E cycle represent principle feature of azobenzene like switchable groups (-N=N-, -CH=N-, C=C) broadly applied for light driven optical switches, nonlinear optical elements, reversible optical storage and other photonics purposes [3]. Despite the fact, that there are promising reviews related to this topic, little few data about the synthesis and characterization of hydantoin (i.e. imidazolidine-2,4-dione) containing substituted benzylidene moiety could be found in the literature. Taking into account mentioned fact, in this article we interpreted preparation and completely structurally characterization of Z-(5-(4-dodecyloxy)benzylidene)imidazolidine-2,4-dione (Figure 1) as potential light-sensitive material. To evaluate the ability of the investigated compound to interact with its environment, the effects of specific and nonspecific interactions on the shifts of absorption maxima were considered by means of the linear solvation energy relationship concepts established by Kamlet-Taft and Catalán.

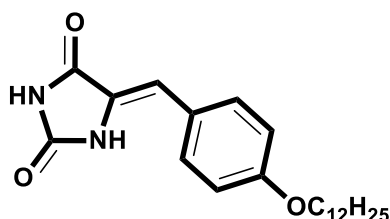
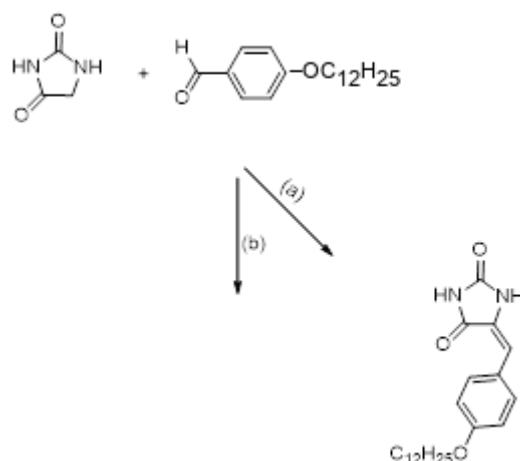


Figure 1. Chemical structure of the investigated Z-(5-(4-dodecyloxy)benzylidene)imidazolidine-2,4-dione

2 Experimental

General

Chemical used in the synthesis of investigated compound were obtained from Sigma Aldrich chemical company and were used without further purification. Solvents used were of spectroscopic grade. Novel Z-(5-(4-dodecyloxy)benzylidene)imidazolidine-2,4-dione was prepared according modified literature procedures [4,5] applying synthesis pathway illustrated on Scheme 1. The IR spectra were recorded using a Bomem MB-Series Fourier Transformer-Infrared (FT-IR) spectrophotometer in the form of KBr pellets. The ¹H and ¹³C NMR spectral measurements were performed on a Bruker AC 250 spectrometer at 400 MHz for ¹H NMR and 100 MHz for the ¹³C NMR. These spectra were recorded at room temperature in DMSO-*d*₆. The ultraviolet-visible (UV-Vis) absorption spectra were recorded on a Shimadzu 1700 spectrophotometer in the region 200–600 nm. The spectra were run in spectroquality solvents (Fluka) using a concentration of 1 x 10⁻⁵ moldm⁻³. All melting points were determined on Electrothermal apparatus and are expressed in degree Celsius. The elemental analysis of the investigated compound was carried out by standard analytical micromethods using an Elemental Vario EL III microanalyzer.



Scheme 1. Reagents and conditions: (a) piperidine, 130 °C; (b) piperidine, 5 min, 200 W.

Synthesis of Z-(5-(4-dodecyloxy)benzylidene)imidazolidine-2,4-dione- method (a):

Imidazolidine-2,4-dione (0.068 mol; 0.68 g) and 4-dodecyloxybenzaldehyde (0.068 mol; 2g) were dissolved in piperidine (5 ml) and heated at 130 °C until the reaction completed. The obtained reaction mixture was poured into lukewarm water (30 ml) and acidified with concentrated HCl. The obtained product was recrystallized from ethanol [4]. M.p. 147 °C, FT-IR (KBr) ν (cm⁻¹): 3217, 3188, 3164, 3153, 3098, 3060, 2950, 2916, 2866, 2848, 1752, 1706, 1652, 1618, 1598, 1532, 1513, 1471, 14233, 1378, 1344, 1316, 1305, 1248, 1199, 1175, 1189, 1088, 10645, 1025, 1013, 955. 935, 919, 879, 853, 825, 805, 740, 722, 592, 535, 526, 515, 498, 469, 457, 449, 444, 238; ¹H NMR (400 MHz, CDCl₃): δ (ppm): 11.03 (s, 1H, NH), 10.22 (s, 1H, NH), 8.18 (d, 2H, J = 5.6 Hz, -C₆H₄-), 7.64 (d, 2H, J = 6.0 Hz, -C₆H₄-), 4.71 (s, 2H, O-CH₂-CH₂-), 3.42 (s, 2H, -C=CH-), 2.17-1.99 (m, 22H, -C₁₂H₂₅-), 1.61 (s, 3H, -C₁₂H₂₅-); ¹³C NMR (100 MHz, CDCl₃): δ (ppm): 166.5 (C2), 160.3, 155.4 (C4), 131.7, 126.7, 126.3, 115.7, 111.4, 68.8, 14.9; Elemental analysis calculated for C₂₂H₃₂N₂O₃ (372.50): C, 70.94, H, 8.66, N, 7.52. Found: C, 70.84, H, 8.76, N, 7.52.

Synthesis of Z-(5-(4-dodecyloxy)benzylidene)imidazolidine-2,4-dione- method (b):

In a microwave vessel, dry piperidine (2 mmol) was added to a mixture of 4-dodecyloxybenzaldehyde (1 mmol; 0.29 g) and hydantoin (1 mmol; 0.1 g). The reaction mixture was then irradiated at 130 °C for 5 min under 200 W microwave power. The mixture was then cooled to room temperature, poured into lukewarm water (30 ml) and acidified with concentrated HCl. The obtained product was recrystallized from ethanol [5].

3 Results and discussion

The main goal of this work was the synthesis of new hydantoin derivative as potential light-sensitive material. The synthesis and spectroscopic characteristics of countless hydantoin derivatives are designated from the literature, but no hydantoin bearing C=C bond as a bridge between this rigid core and p-alkoxy substituted phenyl ring and accordingly its spectroscopic data are published up to now.

In the present work, some recently developed compound containing hydantoin framework, was obtained in good yields by cycloaddition reaction and microwave synthesis (Scheme 1). Z-(5-(4-dodecyloxy)benzylidene)imidazolidine-2,4-dione was completely structurally characterized by melting point, FTIR, NMR, UV-Vis spectroscopy, elemental analysis and thin layer chromatography. The results of FTIR spectroscopy validate the structure of the above-mentioned compound, showing two strong peaks between 3200-3300 cm⁻¹, that were assigned to the NH of the amide and imide imide groups. Absorption bands between 1780 and 1730 cm⁻¹ characterize the asymmetric and symmetric stretching of the carbonyl groups of the hydantoin ring.

The structure of newly prepared compound has also been confirmed by ¹H and ¹³C NMR spectroscopies. The singlets of ¹H NMR spectra at 11.03 ppm and 10.22 ppm, can be assigned to acidic

protons from the amide and imide groups, respectively. The doublets at 8.18 ppm and 7.64 ppm affirmed on *p*-substituted phenyl ring, while singlet at 4.17 ppm pointed on the -CH₂- group from the alkyl chain connected to O-atom. Signals for the rest of the alkyl chain were observed as multiples at 2.17-1.99 ppm. In the ¹H NMR spectrum of the investigated compound, there is a singlet at 3.42 ppm which indicate a -CH- proton from the C=C bond bridging two aromatic rings [6].

3.1 Solvent effects on UV-Vis absorption maxima

The interpretation of the broad bands present in the ultraviolet absorption spectra of many organic compounds in solution is still difficult, and the underlying doubt as to whether or not data relating so such bands are of fundamental significance detracts from the value of any conclusions drawn [7]. UV-Vis absorption spectra of all hydantoin (imidazolidines) whose structures are very close to uracil framework exhibit absorption peaks in the following spectral ranges: 200-250 and 300-400 nm. The first absorption band is attributed to $\pi \rightarrow \pi^*$ transition of N-C=O chromophore and the second to the corresponding transition of carbonyl group. The dissimilarity in peak positions for imidazolidines and their analogs is due to the effect of attached substituents. These spectral characteristics are the most likely the consequence of $\pi \rightarrow \pi^*$ transition of the carbonyl group of the imidazolidine ring rather than $n \rightarrow \pi^*$ transitions of it. This is because the benzene ring coupled with to the rigid hydantoin core produce extensive delocalization in these structures and determines $\pi \rightarrow \pi^*$ transitions.

The UV-Vis absorption spectrum of *Z*-(5-(4-dodecyloxy)benzylidene)imidazolidine-2,4-dione is characterized by two broad bands in the 200-220 nm and 330-350 nm, respectively, regardless of the polarity and acidic/basic properties of the solvent. The higher magnitude of peaks assigned to carbonyl chromophore in position 4 of the imidazolidine ring and greater delocalization of electronic cloud is observed and further analyzed in detail.

Table 1. Absorption maxima of the *Z*-(5-(4-dodecyloxy)benzylidene)imidazolidine-2,4-dione in selected solvent set

Solvent	λ (nm)
1. Chloroform	336.0
2. Dichlormethane	335.0
3. Ethanol	338.0
4. Diethylether	279.0
5. Acetone	331.0
6. Toluene	331.0
7. Acetic acid	341.0
8. Dimethylformamide	333.0
9. Ethylacetate	328.8
10. Methanol	336.0
11. Pyridine	335.4
12. Dimethylsulfoxide	336.0
13. Acetonitrile	330.6
14. 1-Propanol	337.0
15. 1-Butanol	337.0
16. 2-Methyl-2-propanol	338.0
17. <i>N</i> -Methylformamide	335.8
18. Methylacetate	328.8
19. 1,4-Dioxane	331.5
20. <i>N,N</i> -Dimethylacetamide	333.6
21. <i>terc</i> -Butanol	338.0
22. 2-Butanol	338.5

The UV-Vis absorption spectra revealed that the intensity of the absorption band placed in the 330-350 spectral range increases with the enhancing solvent polarity and its acidic properties (Tables 1 and 2) [8]. Because previously reported results clearly confirmed the hypothesis that electron distribution and stereochemistry are important in the establishing interactions between compound and its environment, the effect of solvent dipolarity/polarizability and solvent/solute hydrogen bonding interactions were further analyzed by means of the linear solvation energy relationship concepts proposed by Kamlet-Taft and Catalán. The effects of the nonspecific and specific solvent interactions on the investigated 5-(4-dodecyloxybenzylidene)hydantoin were interpreted using the general solvation equations:

$$\nu_{\max} = \nu_{\max 0} + a\alpha + b\beta + s\pi^* \quad (1)$$

$$\nu_{\max} = \nu_{\max 0} + aSA + bSB + cSP + dSdP \quad (2)$$

and the correlation of the spectroscopic data with solvent parameters was performed by means of multiple linear regression analysis. In both models, the coefficient *a* describes the interactions between the atomic group from the proton-giving solvent (i.e. hydrogen bond donor-HBD) and the corresponding atomic group from the proton-receiving compound (hydrogen bond acceptor-HBA), while the coefficient *b* describes the interactions in forming a hydrogen bond but in the opposite direction. It can be expected that HBD solvents will interact with O-atoms from the carbonyl groups and the alkoxy group through formation a hydrogen bonds of different intensity.

Table 2. Solvent parameters

Solvent	Kamlet-Taft			Catalán			
	π	β	α	SA	SB	SP	SdP
1. Chloroform	0.58	0.00	0.44	0.047	0.071	0.783	0.614
2. Dichloromethane	0.82	0.00	0.30	0.040	0.178	0.761	0.769
3. Ethyl alcohol	0.54	0.77	0.83	0.400	0.658	0.633	0.783
4. Diethyl ether	0.27	0.47	0.00	0.000	0.562	0.617	0.385
5. Acetone	0.71	0.48	0.08	0.00	0.475	0.651	0.907
6. Toluene	0.54	0.11	0.00	0.000	0.128	0.782	0.284
7. Acetic acid	0.64	0.45	1.12	0.689	0.390	0.651	0.676
8. Dimethylformamide	0.88	0.69	0.00	0.031	0.613	0.759	0.977
9. Ethyl acetate	0.55	0.45	0.00	0.000	0.542	0.656	0.603
10. Methyl alcohol	0.60	0.62	0.93	0.605	0.545	0.608	0.904
11. Pyridine	0.87	0.64	0.00	0.033	0.581	0.842	0.761
12. Dimethyl sulfoxide	1.00	0.76	0.00	0.072	0.647	0.830	1.00
13. Acetonitrile	0.75	0.31	0.19	0.044	0.286	0.645	0.974
14. n-Propyl alcohol	0.52	0.90	0.78	0.367	0.782	0.658	0.748
15. n-Butyl alcohol	0.47	0.88	0.79	0.341	0.809	0.674	0.655
16. Isopropyl alcohol	0.41	1.01	0.68	/	/	/	/
17. N-Methylformamide	0.88	0.69	0.00	/	/	/	/
18. Methyl acetate	0.60	0.42	0.00	0.000	0.527	0.645	0.637
19. 1,4-Dioxane	0.55	0.37	0.00	0.000	0.444	0.737	0.312
20. N,N-Dimethylacetamide	0.88	0.76	0.00	0.028	0.650	0.763	0.987
21. terc-Butyl alcohol	0.41	1.01	0.68	0.145	0.928	0.632	0.732
22. sec-Butyl alcohol	0.40	0.80	0.69	0.221	0.888	0.656	0.706

The results of multiple regressions presented in Tables 3 and 4, indicated that the absorption frequencies of the investigated compound in the selected solvent set, showed satisfactory correlation with β , α , π parameters. The negative sign of the coefficient s in the total solvatochromic equations denotes a bathochromic shift with enhancing solvent polarity/polarizability. In accordance with positive solvatochromism of the analyzed compound are the negative signs of regression coefficient a and b implying stabilization of the electronic excited state relative to ground state. The percentage contributions of solvatochromic parameters (Table 3) show that solvatochromism in general is the consequence of solvent acidity and basicity rather than dipolarity/polarizability. These results are in accordance with the preferred existence of hydantoin in the lactam tautomeric form and the literature known hypothesis that hydrogen bonding is an essential factor in forming solute/solvent interactions [9].

As can be seen from the Tables 3 and 4, the values of the correlation coefficient R determined with confidence level of 95% for both models are greater than 0.95. Based on this and other statistical indicators, it can be concluded that the selected equations are suitable for the analysis of the solvatochromism of 5-benzylidene hydantoin derivative. The accuracy of the model in predicting the positions of absorption maxima in different solvents is shown in Figures 2 and 3 by comparing experimentally determined and model-predicted frequencies of the absorption maxima.

Table 3. Regression fits to solvatochromic parameters (1) and percentage contribution of solvatochromic parameters

No.	ν_0 (10^3cm^{-1})	s (10^3cm^{-1})	b (10^3cm^{-1})	a (10^3cm^{-1})	R^a	s^b	F^c	Solvent used ^d	$P\pi^*$ (%)	$P\beta$ (%)	$P\alpha$ (%)
1	30.79 (± 0.18)	-0.32 (± 0.25)	-0.69 (± 0.18)	-0.52 (± 0.15)	0.967	0.098	39	3,5,8,9,13-16, 18-21	20.9	45.1	33.9

^aCorrelation coefficient; ^bStandard error of the estimate; ^cFisher's test; ^dSolvent number as given in Table 1

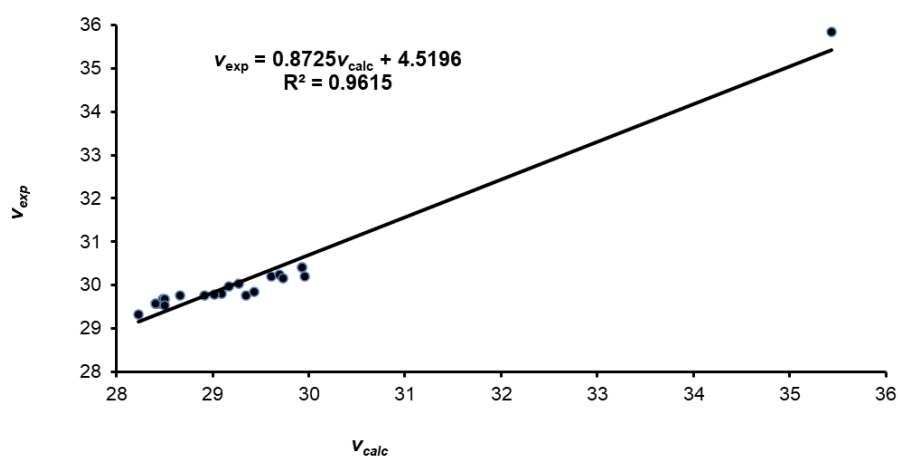


Figure 2. Comparison of experimental frequencies and the frequencies determined by Kamlet-Taft equation.

Table 4. Regression fits to solvatochromic parameters (2)

No.	ν_0 (10^3cm^{-1})	a (10^3cm^{-1})	b (10^3cm^{-1})	c (10^3cm^{-1})	d (10^3cm^{-1})	R^a	s^b	F^c	Solvent used ^d
1	32.09 (± 0.09)	-0.26 (± 0.05)	-2.25 (± 0.24)	-1.57 (± 0.09)	-0.18 (± 0.09)	0.991	0.056	99	5-9,11- 15,18,20

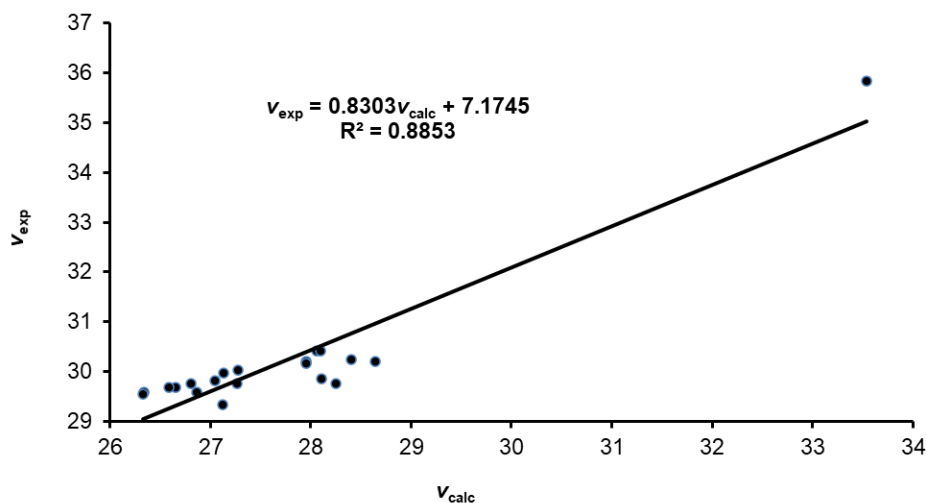


Figure 3. Comparison of experimental frequencies and the frequencies determined by Catalan equation

4 Conclusion

In this work, the classical and microwave-assisted synthesis of Z-(5-(4-dodecyloxy)benzylidene)imidazolidine-2,4-dione has been described. The chemical structure and purity have been confirmed by melting point, FTIR, ^1H NMR, ^{13}C NMR, UV-Vis spectroscopy, elemental analysis and thin layer chromatography. The satisfactory correlation of the ultraviolet absorption frequencies of the investigated Z-(5-(4-dodecyloxy)benzylidene)imidazolidine-2,4-dione with Kamlet-Taft and Catalán general solvatochromic equation indicates that the selected models give a correct interpretation of the linear solvation energy relationships of the complex hydantoin system in the solvents used. This demonstrates that an equation with three or four solvatochromic parameters can be used to evaluate the effects on both types of hydrogen bonding and the solvent dipolarity/polarizability effects for potentially light-sensitive hydantoins. For this reason, it is considered that the results presented in this work may be utilized to quantitatively separate the overall solvent effect into specific and nonspecific contributions using LSER method.

5 References

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