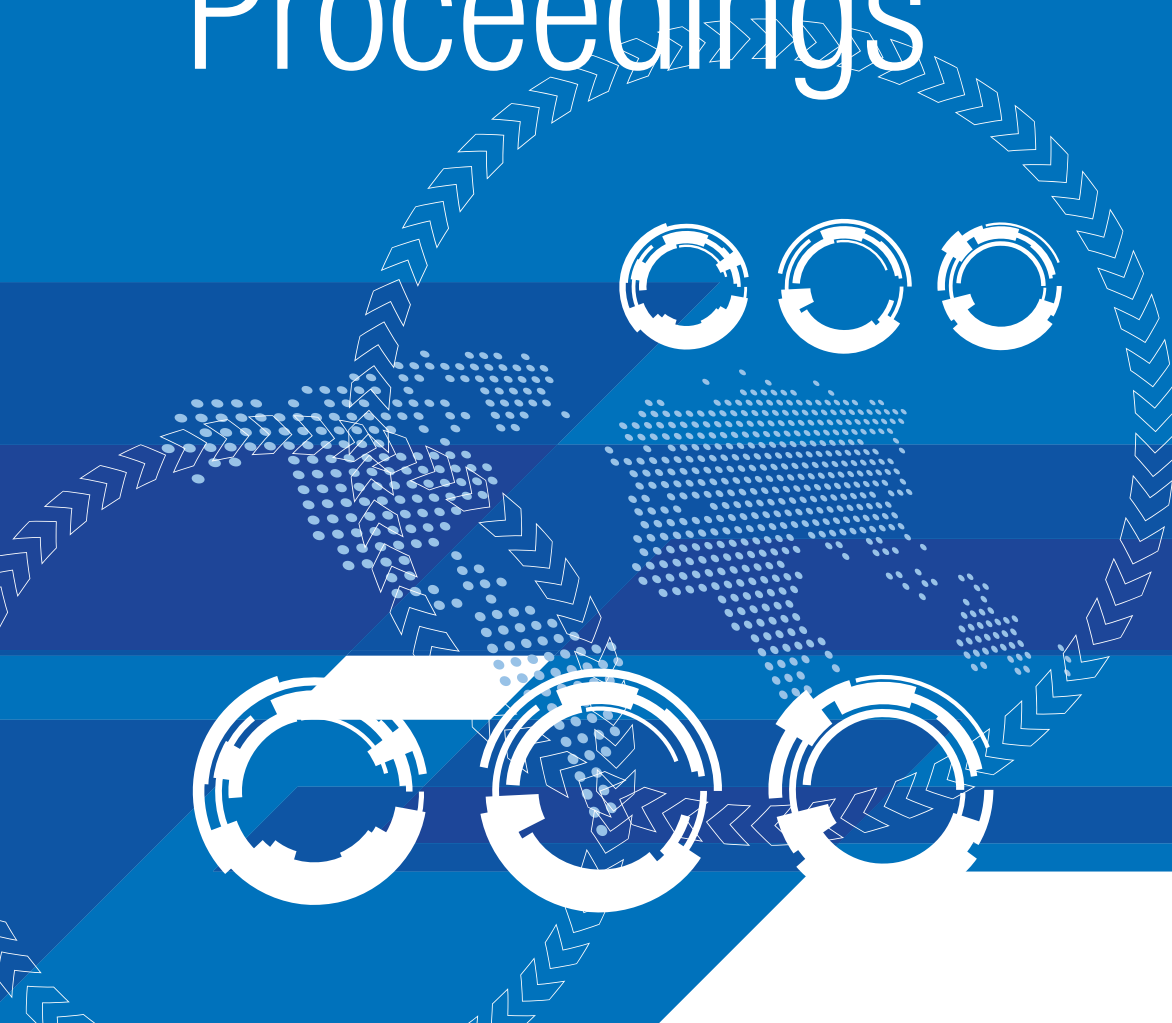




Zbornik radova Proceedings



PROCESING '19

**32. MEĐUNARODNI KONGRES
O PROCESNOJ INDUSTRIJI**

Beograd, 30. i 31. maj 2019.

ZBORNİK RADOVA

**pisanih za 32. Međunarodni kongres o procesnoj industriji
PROCESING '19**



2019

ZBORNİK RADOVA
pisanih za 32. Međunarodni kongres o procesnoj industriji
PROCESING '19

Sava centar, Beograd
30. i 31. maj 2019.

Izdavač

Savez mašinskih i elektrotehničkih
inženjera i tehničara Srbije (SMEITS)
Društvo za procesnu tehniku
Kneza Miloša 7a/II,
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ISBN

978-86-81505-94-6

Tiraž

550 primeraka

Štampa

Paragon, Beograd



Društvo za procesnu tehniku
pri SMEITS-u



Katedra za procesnu tehniku
Mašinskog fakulteta u Beogradu

CIP - Каталогизација у публикацији - Народна библиотека Србије, Београд

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

КОНГРЕС о процесној индустрији ПРОЦЕСИНГ (32 ; 2019 ; Београд)

Zbornik radova [pisanih za 32. kongres o procesnoj industriji] - PROCESING 2019 [Elektronski izvor] : Beograd, 30. i 31. maj 2019. / [organizator Savez mašinskih i elektrotehničkih inženjera i tehničara Srbije (SMEITS), Društvo za procesnu tehniku ; urednici Dejan Radić, Miroslav Stanojević]. - Beograd : Savez mašinskih i elektrotehničkih inženjera i tehničara Srbije (SMEITS), Društvo za procesnu tehniku, 2019 (Beograd : Paragon). - 1 elektronski optički disk (CD-ROM) ; 12 cm

Sistemski zahtevi: Nisu navedeni. - Nasl. sa naslovnog ekrana. - Tiraž 550.
- Bibliografija uz svaki rad. - Abstracts.

ISBN 978-86-81505-94-6

1. Савез машинских и електротехничких инжењера и техничара Србије (Београд). Друштво за процесну технику

a) Машинство - Зборници b) Процесна индустрија - Зборници COBISS.SR-ID 277467660

Održavanje 32. Procesinga finansijski je pomoglo
Ministarstvo prosvete, nauke i tehnološkog
razvoja Republike Srbije



Programski pokrovitelji

■ TEHNOLOŠKO-METALURŠKI FAKULTET UNIVERZITETA U BEOGRADU, BEOGRAD ■ FAKULTET ORGANIZACIONIH
NAUKA UNIVERZITETA U BEOGRADU, BEOGRAD ■ FAKULTET TEHNIČKIH NAUKA UNIVERZITETA U NOVOM SADU,
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U KRAGUJEVCU, KRAGUJEVAC ■ TEHNOLOŠKI FAKULTET UNIVERZITETA U NOVOM SADU, NOVI SAD ■ FAKULTET
ZA MENADŽMENT SREMSKI KARLOVCI, UNIVERZITET „UNION - NIKOLA TESLA“, BEOGRAD ■ DEPARTMAN ZA
ENERGETIKU I PROCESNU TEHNIKU FAKULTETA TEHNIČKIH NAUKA UNIVERZITETA U NOVOM SADU, NOVI SAD
■ INOVACIONI CENTAR TEHNOLOŠKO-METALURŠKOG FAKULTETA UNIVERZITETA U BEOGRADU, BEOGRAD ■
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Gornja Toplica, Popadić

Medijski pokrovitelj



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SOLVATOCHROMIC INVESTIGATION OF PYRIDINE-CONTAINING AZO DYES AS BUILDING BLOCKS FOR MOLECULAR SWITCHES

PROUČAVANJE SOLVATOHROMNIH SVOJSTAVA PIRIDINSKIH AZO BOJA KAO GRADIVNIH JEDINICA ZA MOLEKULSKE PREKIDAČE

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Molecular switches, that are capable of transmitting information in a quick fashion, have an important role in information technologies and have become key components of advanced materials. Namely, molecular switches present small molecules or supramolecular species that can be reversibly shifted between two (or more) stable states possessing different physical features. In this way, they enable complex systems to respond to changes in their environment including changes in light intensity, temperature or voltage. In the present work, five pyridine-containing azo dyes were synthesized with a view to the development of novel molecular switches. The structural features of the investigated dyes were characterized by elemental analysis, FT-IR, ¹H and ¹³C NMR spectroscopy, while their UV/Vis absorption spectra were recorded in twenty solvents of different polarities. To estimate the ability of the investigated dyes to interact with their environment, the effects of solvent dipolarity/polarizability and solvent–solute hydrogen-bonding interactions on the shifts of the absorption maxima were rationalized by means of the linear solvation energy relationship concepts proposed by Kamlet–Taft and Catalán. Based on the analysis of the structural effects on the sensitivity of the investigated dyes to changes in the polarity of their environment, the possible applications of these photoactive materials were further discussed.

Key words: molecular switches; azo dyes; intermolecular interactions; isomerism.

Molekulski prekidači sposobni da brzo prenose informacije imaju važnu ulogu u informacionim tehnologijama, a postali su i ključne komponente naprednih materijala. Naime, molekulski prekidači predstavljaju male molekule ili supramolekulske vrste koji se mogu reverzibilno pomerati između dva (ili više) stabilnih stanja različitih fizičkih svojstava. Na ovaj način oni omogućavaju da kompleksni sistemi reaguju na promene u svom okruženju koje, između ostalog, obuhvataju promene u intenzitetu svetlosti, temperature ili napona. U cilju razvoja novih molekulskih prekidača, pet azo boja koje sadrže piridinsko jezgro je sintetisano u ovom radu i potpuno strukturno okarakterisano primenom elementarne analize, FT-IR, ¹H i ¹³C NMR spektroskopskih metoda. Njihovi UV/Vis apsorpcioni spektri su određeni u dvadeset rastvarača različite polarnosti. Da bi se procenila sposobnost proučavanih boja da uspostavljaju interakcije sa svojim okruženjem, uticaj dipolarnosti/polarizabilnosti rastvarača i vodoničnog vezivanja između molekula rastvarača i rastvorene supstance proučavani su metodama linearne korelacije energije solvatacije prema Kamlet–Taftu i Katalanu. Na osnovu analize uticaja molekulske strukture na osetljivost proučavanih boja na promene u polarnosti okruženja dalje su diskutovane moguće primene ovih fotoaktivnih materijala.

Ključne reči: molekulski prekidači; azo boje; međumolekulske interakcije; izomerizacija.

1 Introduction

Due to the great tunability of their structure and the electronic properties, organic molecules that contain the azobenzene backbone [–Ar–N=N–Ar–] have been identified as promising materials in the field of molecular switches [1]. An external stimulus, usually irradiation with light of a specific wavelength, causes a conversion between two forms, namely the *trans* (*E*) and *cis* (*Z*) isomers of

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different stability. The rearrangement of the electronic and nuclear structure of the molecule occurs in this process without any bond cleavage. The isomerization is reversible and the thermodynamically stable *trans* (*E*) isomer can be restored in the dark in a quick fashion.

Herein, we report the synthesis and characterization of five pyridine- and pyrimidine-containing azo dyes with emphasis on the structural considerations and the patterns of intermolecular interactions in solution. It is shown that the stronger push–pull configuration of these dyes results in faster isomerisation rates and, therefore, opens up perspectives for various applications in many devices, such as systems for opto-electronics, holographic materials and multicolor displays [2]. With this regard, we wanted to examine how the pyridine/pyrimidine moiety and various substituents affect the chromophoric π -electron system as a result of intermolecular interactions with their environment. The UV/Vis absorption spectra of the investigated dyes were measured in the range from 300 to 600 nm in twenty solvents. The effects of solvent dipolarity, polarizability and solvent–solute hydrogen bonding on the shift of the absorption maxima were evaluated by means of the linear solvation energy relationship (LSER) model of Kamlet and Taft [3], given by Eq. 1:

$$\nu = \nu_0 + s\pi^* + a\alpha + b\beta \quad (1)$$

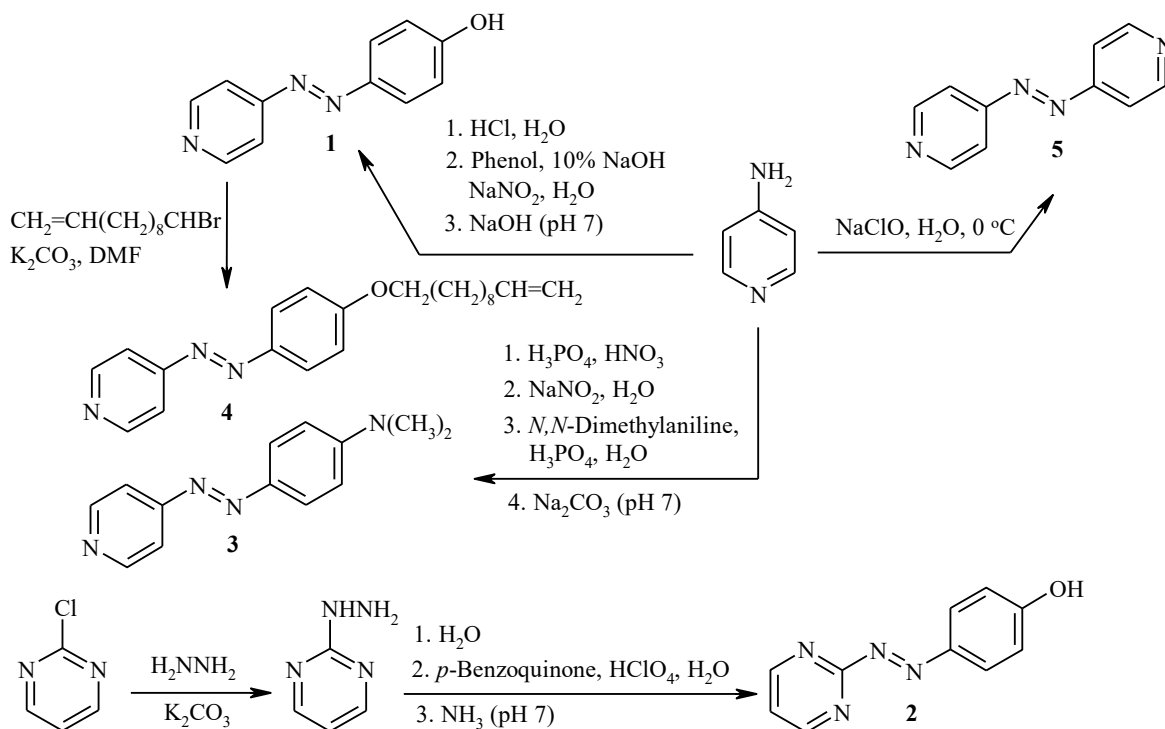
where α describes the hydrogen bond-donating ability, β the hydrogen bond-accepting ability, and π^* the dipolarity/polarizability of a solvent.

The effects of different intermolecular interactions on the shift of the absorption maxima of the synthesized dyes were additionally interpreted by using the LSER model of Catalán [4], given by Eq. 2:

$$\nu = \nu_0 + aSA + bSB + cSP + dSdP \quad (2)$$

where SA, SB, SP and SdP characterize acidity, basicity, polarizability and dipolarity of a solvent, respectively.

2 Experimental



Scheme 1 Synthesis of the investigated pyridine- and pyrimidine-containing azo-dyes

All compounds were prepared according to adapted literature procedures (Scheme 1, [5–7]). The FTIR spectra were recorded using a Bomem MB series 100 spectrophotometer in the form of KBr pellets. The ¹H and ¹³C NMR spectral measurements were performed on a Bruker AC 250

spectrometer at 200 MHz for the ^1H NMR and 50 MHz for the ^{13}C NMR spectra. These spectra were recorded at room temperature in DMSO- d_6 . The UV/Vis absorption spectra were measured with a Shimadzu 1700 spectrophotometer. The elemental analyses of the investigated compounds were carried out by standard analytical micromethods using an Elemental Vario EL III microanalyzer.

3 Results and Discussion

The investigation of the solvatochromic properties of the synthesized azo dyes was performed in twenty solvents of different polarity and hydrogen bonding capacity. The used solvents covered a wide range of properties with a large variance. The UV/Vis absorption spectra of the dyes showed an intense band in the region from 340 to 540 nm and a broad, weak band in the low-energy region. Overall, as the solvent polarity increases from dioxane to acetic acid (Table 1), the UV/Vis absorption spectra of dyes **1–4** showed a large bathochromic shift of the main UV/Vis band. Dye **5** did not show a significant solvatochromic behaviour.

Table 1 The absorption maxima of the investigated compounds **1–5** in selected solvents

Solvent Comp. No.	λ_{max} [nm]				
	1	2	3	4	5
Acetone	352	342	433	353	- ^a
Acetonitrile	351	342	434	353	282
1-Butanol	364	364	440	360	285
Butanone	351	-	433	355	- ^a
Dioxane	349	342	426	352	295
Dimethyl sulfoxide	364	353	451	359	284
Ethanol	362	365	440	359	284
Ethyl acetate	352	337	428	352	284
Formamide	361	363	457	360	291
Ethylene glycol	364	367	460	363	287
Chloroform	344	350	436	358	287
Methanol	360	360	442	359	283
<i>N</i> -Methylformamide	361	360	443	359	289
<i>N,N</i> -Dimethylformamide	361	347	442	358	285
Pyridine	364	353	442	358	- ^a
1-Propanol	364	366	440	359	284
2-Propanol	365	363	437	357	285
<i>tert</i> -Butyl alcohol	364	361	432	356	285
Tetrahydrofuran	356	340	432	356	287
Acetic acid	392	370	536	387	287

^a In the solvent absorption range.

The results of the multiple linear regression analysis using the Kamlet–Taft and Catalán parameters are given in Tables 2 and 3. The statistical parameters indicated that the used multiparameter equations were valid and gave significant information on the solvatochromic behavior of the investigated azo dyes.

Table 2 Regression fits to solvatochromic parameters (Eq. (1))

Compound	ν_0 [cm ⁻¹]	a	b	s	R^a	sd^b [cm ⁻¹]	F^c	n^d
1	29798 (±203)	-339 (±119)	-1704 (±178)	-1028 (±224)	0.952	173	48	19 ^e
2	30393 (±318)	-1861 (±167)	-946 (±262)	-1112 (±347)	0.958	267	56	20
3	24781 (±143)	-795 (±80)	-219 (±120)	-2320 (±158)	0.975	115	90	18 ^f
4	28980 (±171)	-386 (±87)	-425 (±168)	-791 (±161)	0.895	120	19	18 ^g

^aCorrelation coefficient; ^bStandard error of the estimate; ^cFisher's test; ^dNumber of the solvents in the set; ^eAcetic acid was excluded from the correlation set; ^fAcetic acid and *N*-methylformamide were excluded from the correlation set; ^gAcetic acid and chloroform were excluded from the correlation set.

Table 3 Regression fits to solvatochromic parameters (Eq. (2))

Compound	ν_0 [cm ⁻¹]	a	b	c	d	R^a	sd^b [cm ⁻¹]	F^c	n^d
1	31490 (±384)	-737 (±148)	-2172 (±175)	-2334 (±458)	-666 (±194)	0.974	136	61	18 ^e
2	30808 (±1121)	-2819 (±397)	-1430 (±514)	-1572 (±1390)	f	0.901	418	20	18 ^g
3	26421 (±191)	-1190 (±74)	-214 (±87)	-3500 (±228)	-1023 (±96)	0.992	67	203	18 ^e
4	29764 (±251)	-692 (±93)	-606 (±137)	-1407 (±290)	-318 (±128)	0.955	85	31	17 ^h

^aCorrelation coefficient; ^bStandard error of the estimate; ^cFisher's test; ^dNumber of the solvents in the set. ^eAcetic acid and *N*-methylformamide were excluded from the correlation set. ^fParameter is not statistically significant; ^g*N*-methylformamide and butanone were excluded from the correlation set; ^hAcetic acid, *N*-methylformamide and chloroform were excluded from the correlation set.

The results of the LSER analysis indicated that dyes 1–4 are more dipolar in the excited states than in the ground states (the negative s and SP terms). The effect of the dipolarity/polarizability on the shift of the UV/Vis absorption maxima dominates over that of the hydrogen bond capacity. Thus, the UV/Vis absorption maxima undergo a bathochromic shift with increasing the solvent hydrogen bond capacity, as shown by the negative a , b , SA and SB terms. As expected, acetic acid was excluded from the correlation set in most cases, because a large bathochromic shift of dyes with the pyridine moiety results from acid-base interactions, *i.e.*, protonation of the pyridine ring. This effect can make interpretation of the solvatochromism ambiguous.

4 Conclusions

The solvent effects on the position of the UV/Vis absorption maxima depend on the nature (polarity, basicity and steric effects) of the substituent introduced in the *para* position relative to the azo group. With increasing solvent dipolarity/polarizability, the UV/Vis absorption maxima shift bathochromically. The stronger the electron-donating effect of the substituent, the larger the extent of the solvatochromic effect induced by the hydrogen bonding capacity of the solvent. When the solvent has acidic properties, competing acid-base interactions also take place. The investigated dyes fulfil requirements to be additionally used as solvent polarity indicators.

Acknowledgment

Financial support of the Ministry of Education, Science and Technological Development of the Republic of Serbia (Grant No. OI172013) is gratefully acknowledged.

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