Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl19

Spectral Data Base on Photochromic Organic Compounds

Anton O. Ait [a], Valery A. Barachevsky [a], Michael V. Alfimov [a] & Igor I. Baskin [b]

[a] Institute of Chemical Physics RAS, Moscow, Russia.

[b] Institute of Organic Chemistry RAS, Moscow, Russia.

Version of record first published: 24 Sep 2006

To cite this article: Anton O. Ait, Valery A. Barachevsky, Michael V. Alfimov & Igor I. Baskin (1997): Spectral Data Base on Photochromic Organic Compounds, Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals, 298:1, 271-275

To link to this article: http://dx.doi.org/10.1080/10587259708036171

Mol. Cryst. Liq. Cryst., 1997, Vol. 298, pp. 271–275
Reprints available directly from the publisher
Photocopying permitted by license only

SPECTRAL DATA BASE ON PHOTOCHROMIC ORGANIC COMPOUNDS

ANTON O. AIT, VALERY A. BARACHEVSKY, MICHAEL V. ALFIMOV
Institute of Chemical Physics RAS, Moscow, Russia.

IGOR I. BASKIN
Institute of Organic Chemistry RAS, Moscow, Russia.

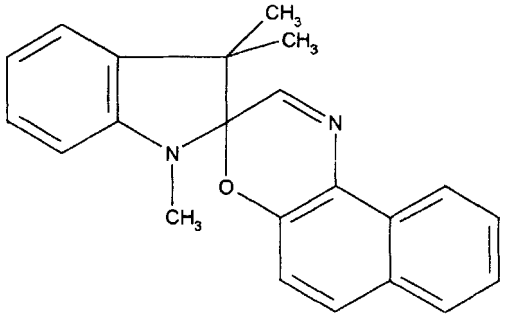
Abstract A data base containing properties and chemical structures of photochromic organic compounds along with the UV and visual absorption spectra of both initial and photoinduced forms has been created. This data base improves efficiency of basic researches for the structure-property relationships.

INTRODUCTION

For the first time a specialized data base containing chemical structure properties of photochromic organic compounds and the UV and visual absorption spectra of initial and photoinduced form has been created. Nowadays, photochromic compounds assume great importance in the fields of high phototechnologies[1-6]. The developed data base improves the efficiency of basic researches for the structure-property relationships, such as the rise in of photochromic compounds up to irreversible photochemical transformations, which hindered their wide use in the science and technique field.

STRUCTURE AND PURPOSES OF THE DATA BASE

The data base consists of two parts: (1) data base on chemical structures and properties of chemical compounds and (2) data base on absorption spectra of the initial and the photoinduced forms of photochromic compounds. In addition to the generalization of gathered information on structures, spectra and properties of photochromic organic compounds, the purpose of the data base is to build data base that could provide a means for assessing the ways of increasing the reversibility of photochromic conversions, changing the spectral characteristics of initial and



CAT.NO	1
Class of compounds	Spirooxazine
Formula	$C_{22}H_{20}N_2O$
Mol. weight	328.4175
Melting Point, °C	117.0 - 119.0

Chemname: 1,3,3-trimethylspiro(indolino-2.3'-3H-naphtho[2.1-b][1.4]oxazine]

λmax CF,nm	Color	ε CF, 1/(M×cm) ×0.001	Medium	T, °C	Comment	Ref
294		4.20	toluene			128
319		4.20	toluene			128
350		4.20	toluene			128

λmax OF,nm	Color	ε OF, 1/(M×cm) ×0.001	Medium	T, °C	Comment	Ref
594		19.00	toluene	20.0	c=0.0002M	128
590		1.85	toluene	20.0	c=0.0002M	128
590		9.80	toluene	20.0	c=0.0002M	63

Fluor.λmax CF,nm	Medium	T, °C	Ref

Fluor.λmax OF,nm	Medium	T, °C	Ref

Quant.yield CF	Medium	T, °C	Ref
0.05			141

Quant.yield OF	Medium	T, °C	Ref
0.23	toluene		146
0.41	methylcyclo-hexane		121

Character of photodegradation

v= 27(I=4x10(17) quant., without filter, toluene);
v=54000(I=4x10(17) quant., glass, "a vitre", toluene);
v=489 (I=4x10(17) quant., glass wood, toluene);
v=900(I=3x10(17) quant., glass wood, toluene)

Activ.Energy,kJ/mol	Medium	Ref
71.00	methylcyclohexane	121
81.00	ethanol	121
112.00	acetonitrile with Na+	
88.00	membrane	60

Decolor Time, s	K, (1/s)	A_0	Medium	pH	T, °C	Ref
	0.54	1.0800	toluene		25.0	146
	0.70		dioxane		25.0	146
	4.40		hexachlorbutane		25.0	49
	1.60	1.0000			25.0	41
	19.10		hexachlorbutane		100.0	105
	2.00		benzonitrile		100.0	105
	0.11		acetonitrile with K+		8.0	134

FIGURE 1 Phisico-chemical and spectral properties of photochromic compounds.

photoinduced forms, the life time of the photoinduced forms and the efficiency of reversible photoconversions.

Besides the spectral-kinetics parameters and the bibliography, the database contains 3D-models of initial and photoinduced forms optimized using semi-empirical quantum-chemical methods. The 3D-models allows, in particular, to calculate the appropriate absorption spectra when lacking experimental data.

The database contains information on photochromic organic compounds from several classes, representing the greatest interest at the moment, namely spiropyran, spirooxazine, chromene and ariloxiquinone.

In connection with creating polymer photochromic glasses, the intensive researches are being conducted in the field of synthesis and study of properties of spirooxazines and chromenes . In their stable forms, spirooxazines and chromenes are colourless, however under the action of the UV light they become colored, displaying a absorption bands of the photoinduced and the stable forms in ranges 540-610 nm and 420-520 nm, respectively. Mixing these compounds at determined ratio makes it possible to receive photochromic materials with neutral coloring of the photoinduced form.

The special interest to ariloxiquinones is connected with the fact that they have thermodynamically stable states for both initial and photoinduced form. This property provides opportunity for using these compounds in the development of recording media for operative optical memory of superhigh resolution.

The data base containing chemical structure and properties of chemical compounds is based on the software shell ISIS/Base operating in Windows 3.x systems. Input and storage of spectra are performed using our original software also operating in Windows 3.x and interacting with ISIS/Base.

One of the screen forms of the part of the data base dealing with phisico-chemical properties of photochromic compounds is shown in Figure 1. Figure 2 depicts screen form with 3D model of both stable and photoinduced form. Finally, screen display of the spectral information contained in the data base is shown in Figure 3.

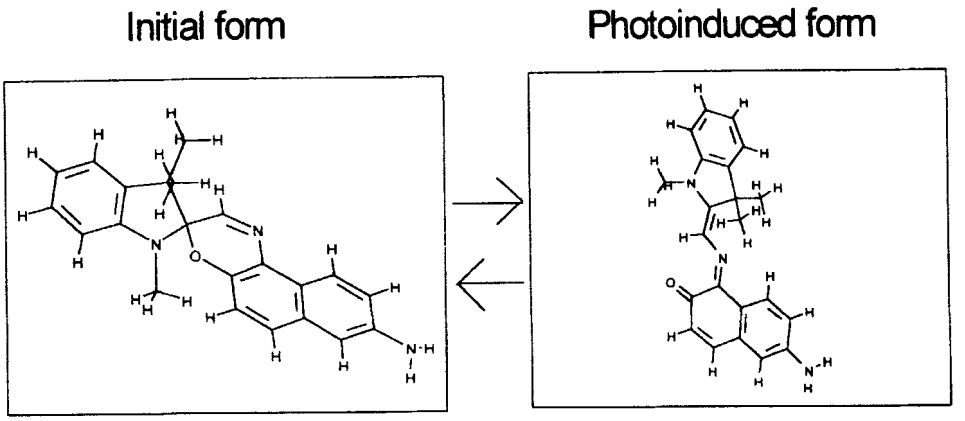


FIGURE 2 3D models of initial and photoinduced forms of 8'-Amino-1,3,3-trimethylspiro-[indoline-2,3'-3H-naphtho[2,1-b] [1,4]oxazine].

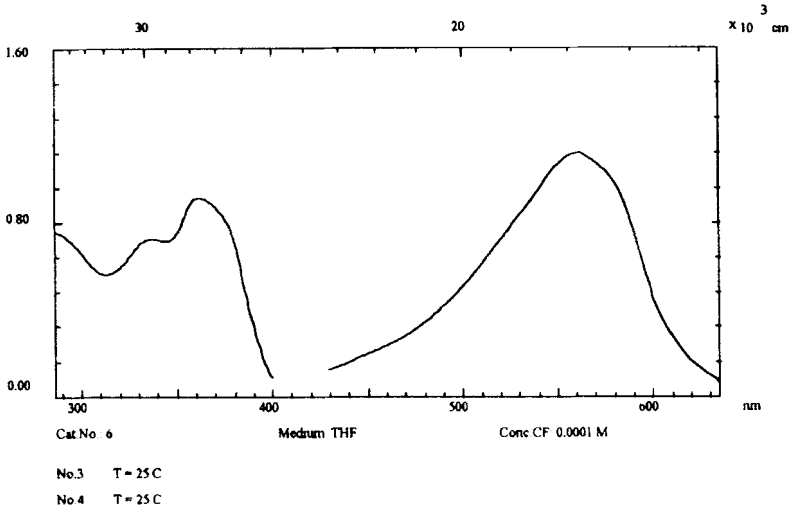


FIGURE 3 Display of absorption spectra of initial and photoinduced forms of 8'-Amino-1,3,3-trimethylspiro-[indoline-2,3'-3H-naphtho[2,1-b] [1,4]oxazine].

CLIENT/SERVER SYSTEM

A client/server system, based on the use of the Dynamic Data Exchange (DDE) mechanism in the framework of the Microsoft Windows environment, has been developed in order to (1) link factographic and literature information on photochromic

organic compounds contained in the ISIS/Base data base with spectral information stored and processed by the SpectrDB program; (2) build 3D (geometrical) models of both closed and open forms from the structural formulae (2D) of the closed form; (3) provide possibility for easy computing of physico-chemical and spectral properties of photochromic compounds contained in the data base using molecular mechanics and semi-empirical quantum mechanics approaches. The client/server system consists of 4 components: (1) the main client program Photochrom controlling the whole course of calculations in all components of the system; (2) the ISIS/Base program (MDL Information Systems, Inc.) for processing information contained in the data base and a special PL program, working in the ISIS/Base environment and providing the client/server features of this component; (3) the original server SpectrDB program for handling spectral data bases; (4) the server HyperChem program (Hypercube, Inc.) for making molecular mechanics and semi-empirical quantum mechanics calculations.

Physico-chemical parameters, such as the heat of formation, energies of highest occupied and lowest unoccupied molecular orbitals can be used to assess relative stabilities of different photochromes or different forms of one photochrome, their ionization and reduction potentials. The possibility for computing absorption spectra is necessary for predicting spectral characteristics of this type of molecules.

REFERENCES

1. V. A. Barachevsky, G. I. Lashkov, V. A. Tsekhovsky, Photochromism and Its Applications (Khimia, Moscow, 1977), p. 277.
2. Photochromism. Technics of Chemistry, edited by G. H. Brown (Wiley Interscience, London, 1971).
3. Photochromism: Molecules and Systems, edited by H.Duerr, H. Bouas-Laurent (Elsevier, Amsterdam, 1990).
4. J. C. Crano, W. S. Kwak, C. N. Nelch, in Photochromic Polymer Systems, edited by C. Mc. Ardle (Blackie, Glasgow, 1992).
5. V. A. Barachevsky. Opt. Memory Neural Networks, 4, 43 (1995).
6. V. A. Barachevsky. Mol. Cryst. Liq. Cryst., 246, 95 (1994).