STUDY OF MAGNETO-OPTICAL PROPERTIES OF AROMATIC LIQUIDS AND THEIR APPLICATION IN SIGNAL PROCESSING

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Abstract. Experimental results of Faraday rotation spectra in the range of 1.8-3.65 eV were obtained for H_2O, CCl_4, dimethylaniline, benzene, nitrobenzene, o-toluidine, o-anisidine, m-chloroaniline and o-chloroaniline. Semi-empirical quantum mechanical self-consistent field (SCF) calculations using the MNDO/D method for organic molecules were chosen to evaluate electronic spectra in the visible range for interpretation of experimental results. It is shown that the magneto-optical response of samples varies not only depending on geometry. distribution of pi electrons in aromatic liquids, but also significantly depends on their chemical composition.

Keywords: *Faraday effect, liquid magneto-optical waveguide logic gates*

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INTRODUCTION

Nowadays, organic materials, both in solid and liquid phases, have been increasingly used in applications. In order to determine the magneto-optical parameters of organic hydrocarbons, experimental studies of aromatic hydrocarbons in the visible region of the spectrum were carried out. Benzene and its derivatives are the basis of many synthesized polymers used in modern devices and are very attractive for research.

The condition of aromaticity is the presence of π-bonds located in the ring structure of molecules, and each atom of the ring must possess *p-orbitals* forming overlapping regions of p_z*-components*. The ring atoms in this case are most often hybridized to the sp^2state . For example, in benzene, all three π-bonds are located within a ring of six atoms in sp^2, which form overlapping $p_z$orbitals [1-4].

This molecule remains a flat ring (with rays of hydrogen atoms) despite torsional deformations and, moreover, satisfies Hückel's rule and, accordingly, is aromatic. NMR experiments with benzene molecules show that delocalized electrons of benzene molecules under the influence of magnetic create an induced ring current *π-electrons*.

Actually, it is precisely this behavior of electrons of the benzene ring and its mono- and di- substituted derivatives that leads to a sufficiently large magneto-optical goodness of organic materials, so these samples were chosen for a more detailed study by the authors of [5, 6].

The magneto-optical Faraday effect chosen for studies of organic liquids occurs when a plane-polarized light wave interacts with matter in the presence of a magnetic field. Light after passing through the sample generally becomes elliptically polarized with the principal axes rotated by some angle relative to the plane of polarization of the incident beam. Under the influence of a relatively weak external field H, the Faraday rotation can be considered as a first-order H effect.

Samples of aromatic liquids with benzene rings: benzene, nitrobenzene, ortho-toluidine, ortho-anisidine, and meta- and ortho-chloraniline were purified by distillation and placed in Wood tubes. The spectral magneto-optical properties of the samples were studied using an MDR12 monochromator, and measurements of the magneto-optical Faraday effect spectra in the wavelength range of 350-600 nm were made. The block diagram of the setup is shown in Fig. 1 [7].

The magneto-optical spectra were studied on a specially selected series of samples to determine the influence of the chemical composition and geometry of molecules on the magnitude of the Faraday effect in the visible region. As was to be expected, the composition of atoms in mono- and di- substituted benzene derivatives has a rather noticeable influence on both optical and magneto-optical properties of the studied liquids (Fig. 2). Comparing the experimental curves of spectral dependences of the Faraday effect for benzene ($C_{(6)\ H6}$) and nitrobenzene ($C_{(6)\ H5}NO_{(2)\ )}$, it is easy to see that the substitution of one hydrogen atom by the $NO_{2,}$group leads to a strong decrease in the maximum of the Faraday effect. The shape of the dispersion curve also changes, as can be seen in Fig. *2a*.

The results of computer calculations in Table 1 [7,8] show that the transition from $C_{(6)\ H6}$to $C_{(6)\ H(5)}NO_2$results in a strong redistribution of electron densities of molecules, and at the same time their energy spectrum changes, the wavelengths of transitions in the table are given in electron-volts (eV) (see the lower calculated curves for the forces of oscillators in Fig. *2a*).

Fig. *2b* shows the spectral curves of the Faraday effect for ortho-anisidine and ortho-toluidine, in which one hydrogen atom of the benzene ring is substituted with the

CH_3O group in o-anisidine and CH_3in o-toluidine, and the second substituents (NH_2) are the same. The presence of an extra oxygen atom leads to the fact that the magneto-optical goodness of o-anisidine is significantly larger than that of o-toluidine.

It was of interest to find out how the structural isomerism due to the different position of di-substituent groups of the benzene skeleton affects their magneto-optical properties. For this purpose, samples of chloraniline in ortho- and meta- states were selected. The results obtained for these samples are presented in Fig. 3.

The magneto-optical spectra were studied on a specially selected series of samples to determine the influence of the chemical composition and geometry of molecules on the magnitude of the Faraday effect in the visible region. As one would expect, the composition of atoms in mono- and di- substituted benzene derivatives has a rather noticeable influence on both optical and magneto-optical properties of the studied liquids. The results of the Faraday rotation spectra for the selected samples in the range of 1.8 - 3.65 eV for a sample layer thickness of 2.3 cm and an applied external magnetic field $H_z = 40$ E are presented in Fig. 4.

The analysis of the obtained data shows that the energy spectra of the studied molecules are strongly influenced not only by the chemical composition, but also by the very location of substituent groups relative to each other. This influence on the magneto-optical properties of the isomers is even more noticeable.

According to the results of the study of magneto-optical spectra shown in Fig. 3, we can conclude that the magneto-optical goodness of organic liquids is quite sufficient for their use in applied purposes, which allows us to formulate the problem for the development of the obtained experimental results for the design of a wide range of devices for processing, storage, and transmission of information [9].

Another interesting application is certainly the choice of using aromatic liquids for data processing such as matrix to matrix multiplication and others. The work in [9] shows how we can utilize magneto-optical advantages for signal processing. For example, we can use the polarization properties of photons and their entanglement to model elementary half-summing.

The purpose of this paper is rather to formulate magneto-optical challenges related to the application of aromatic liquids in modern communication and data storage applications, rather than to explain in detail their entire behavior. The most realistic devices are magneto-optical fibers and the choice of using magneto-optics for controlled OR and NOT gates for data processing [10-13]. Here we will only briefly summarize some ideas of such applications.

Let us perform some elementary calculations for a solenoid magnet, using a fiber 1 centimeter long and 100 μm in diameter with an outer diameter and a core filled with a suitable aromatic liquid as a sample for a magneto-optic device. If we apply a current of about 0.1 A to a 0.2 mm diameter wire coil (with a magneto-optic fiber having the above parameters), the Faraday effect can be adjusted in the range of 30°-45° (angular) depending on the nature of the sample. This means that we can use such organic materials for communication purposes as magneto-optic modulators and insulators without much trouble.

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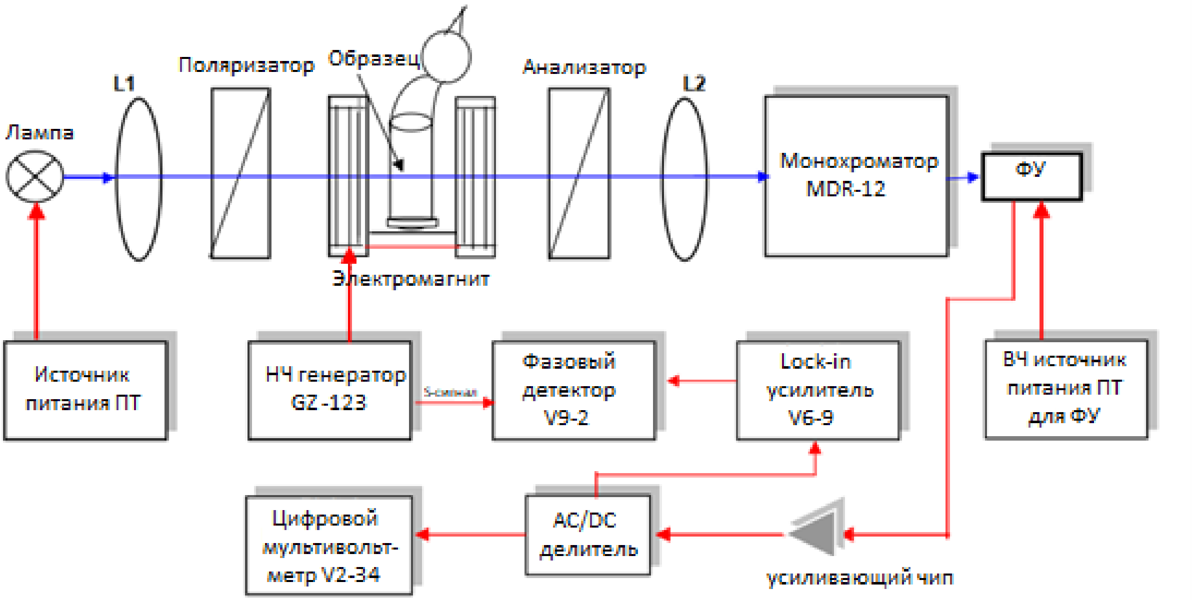
PICTURE CAPTIONS

Fig. 1. Block diagram of the magneto-optical setup for the study of magneto-optical spectra of aromatic liquids.

Fig. 2. Magneto-optical spectra and force calculations of oscillator spectra of disubstituted benzene: benzene and nitrobenzene (a), o-anisidine and o-toluidine (b). The structure of the molecules is at the top.

Fig. 3. Magneto-optical Faraday rotation spectra for o-chloroaniline (*a*, curve 1) and m-doraniline (*a*, curve 2) and their calculated energy spectra (b, c) (without taking into account the effect of the magnetic field).

Fig. 4. Faraday effect in some liquids.



Эксперимент проведён с модуляцией внешнего магнитного поля с частотой f = 37 Гц, H(max) = 40 Э.

Fig. 1.

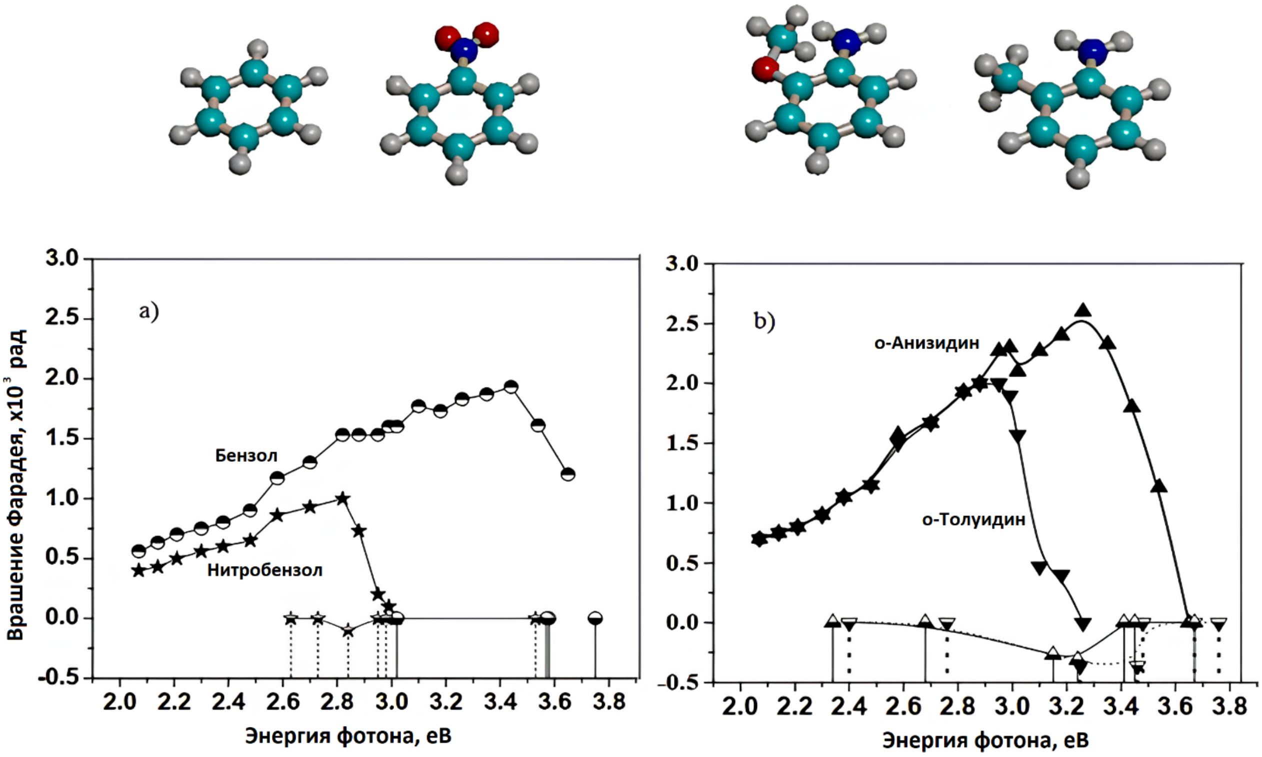
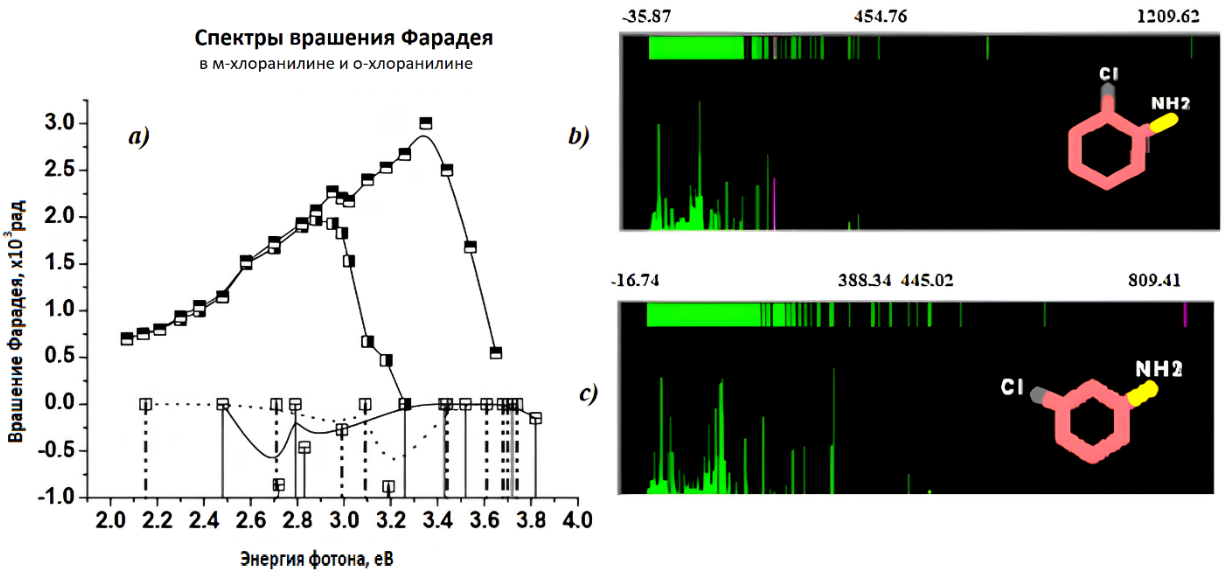
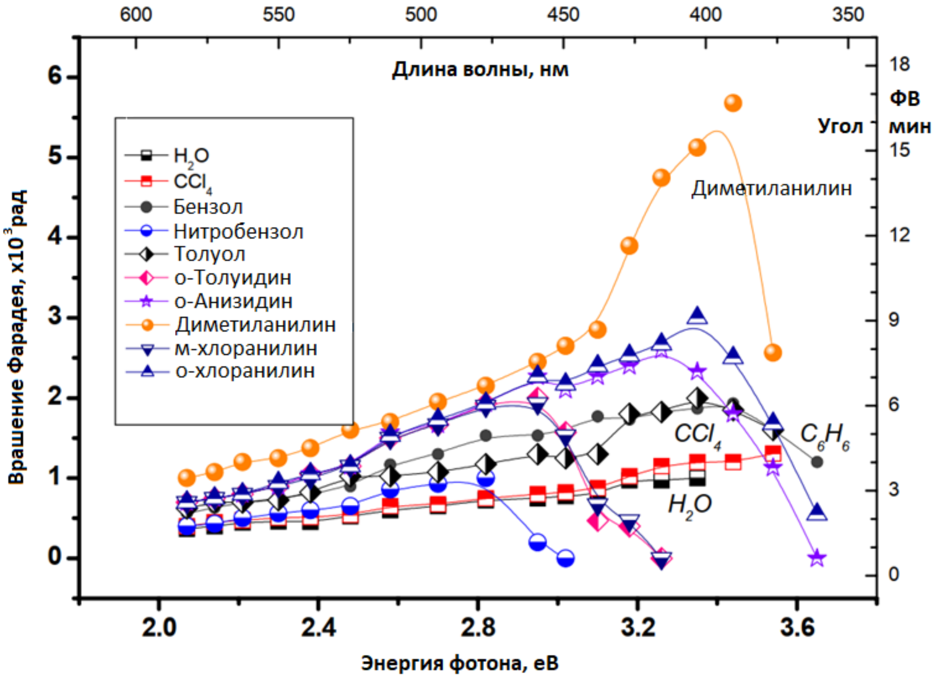


Fig. 2.



Спектры вращения Фарадея
в м-хлоранилине и о-хлоранилине
a)
b)
c)
Вращение Фарадея, x10³рад
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
2.0
2.2
2.4
2.6
2.8
3.0
3.2
3.4
3.6
3.8
4.0
Энергия фотона, eB
-35.87
454.76
1209.62
Cl
NH2
-16.74
388.34
445.02
809.41
Cl
NH2

Fig. 3.



600
550
500
450
400
350
Длина волны, нм
H₂O
CCl₄
Бензол
Нитробензол
Толуол
о-Толуидин
о-Анизидин
Диметиланилин
м-хлоранилин
о-хлоранилин
Угол
ФВ
мин
18
15
12
9
6
3
0
Диметиланилин
CCl₄
C₆H₆
H₂O
Вращение Фарадея, x10³рад
6
5
4
3
2
1
0
2.0
2.4
2.8
3.2
3.6
Энергия фотона, eB

Fig. 4.

Table 1. Electronic spectra of aromatic molecules (based on MNDO/d calculations).

Benzene	687.04	410.77	410.77	346.28	346.28	330.63	292.48						
Transition	1	2	3	4	5	6	7						
Degeneracy	1	2	2	2	2	1	2						
Spin multiplicity	3	3	3	3	2.002	1	3						
Oscillator strength	0	0	0	0	0	0	0						
Nitrobenzene	2270.7	1344.68	1078.19	922.14	658.77	464.54	454.08	427.43	416.62	412.32	411.83		
Transition	1	2	3	4	5	6	7	8	9	10	11		
Degeneracy	1	1	1	1	1	1	1	1	1	2	2		
Spin multiplicity	3	3	1	1	1	3	3	1	3	3	1		
Oscillator strength	0	0	0	0	0	0	0	0.001	0	0	0		
o-Toluidine	740.34	515.65	448.86	381.81	357.99	356.79	338.25	329.37					
Transition	1	2	3	4	5	6	7	8					
Degeneracy	1	1	1	1	2	2	1	1					
Spin multiplicity	3	3	3	1	1	3	3	3					
Oscillator strength	0	0	0	0.036	0.036	0	0	0					
o-Anizidine	826.81	529.61	463.15	394.1	382.97	363.53	359.02	337.44	256				
Transition	1	2	3	4	5	6	7	8	12				
Degeneracy	1	1	1	1	1	1	1	1	1				
Spin multiplicity	3	3	3	1	1	3	3	3	1				
Oscillator strength	0	0	0	0.027	0.031	0	0	0	0.299				
m-Chloraniline	770.64	577.72	457..35	415.29	401.34	388.63	360.3	343.76	337.08	335.35	331.81	303.57	280.1
Transition	1	2	3	4	5	6	7	8	9	10	11	12	13
Degeneracy	1	1	1	1	1	1	1	1	2	2	1	1	1
Spin multiplicity	3	3	3	1	3	1	3	3	3	1	3	3	1
Oscillator strength	0	0	0	0.027	0	0.088	0	0	0	0	0	0	0.498
o-Chloraniline	1153.7	723.24	500.98	455.06	444.09	437.58	379.92	361.87	352.53	333.63	324.96	290.72	
Transition	1	2	3	4	5	6	7	8	9	10	11	17	
Degeneracy	1	1	1	1	1	1	1	1	1	3	1	1	
Spin multiplicity	3	3	3	1	3	1	3	3	3	1	1	1	

Oscillator strength	0	0	0	0.086	0	0.046	0	0	0		0.015	0.272