THE ABSORPTION BAND INTENSITY OF THE IR - SPECTRUM OF THE
o - TOLUNITRILE MOLECULE

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The theoretical study of absorption bands intensities of the IR-spectrum of the o-tolunitrile molecule has been conducted by the method of the theoretical oscillatory spectroscopy. Theoretical values of absorption bands intensities of the IR - spectrum of the molecule have been received, the set of electrooptical parameters has been found, the analysis of the creation nature of each absorption band has been carried out and the theoretical curve of the spectral distribution of the absorption coefficient of the o-tolunitrile molecule has been plotted.

Vibration of polyatomic molecules are directly manifested in infrared absorption spectra of appropriate molecules. The absorption process takes place as a result of interaction of the electron and nucleus of the molecule with the electromagnetic field of the light waves. The electron shell of the molecule deforms at the nuclear vibrations. The character of these deformations depends both on the shell's structure and on the oscillation properties. Peculiarities of the structure of the electron shell of the molecule are completely manifested in intensities and polarizations of spectral lines and bands. Exploring intensities and polarizations in oscillatory spectra, we may get the information about parameters, characterizing the electron shell of the molecule. Firstly, it is dipole moments and polarizabilities of separate bonds and their derivatives on oscillatory coordinates.

On a level with the application of quantum mechanics apparatus to the task of intensities of the oscillatory absorption spectrum, giving still some divergence from the experiment because of the polyatomic molecules composition complexity, a valence-optic theory [1] is the most real base for the theoretical study of intensities in infrared absorption spectra of polyatomic molecules.

Given work is devoted to the calculation of intensities of the absorption IR-spectrum of the o-tolunitrile molecule by means of the program, created on the base of the valence-optic theory [2]. Calculations, according to this program, allow not only to calculate values of integral intensities of IR-absorption bands of molecules and to find electrooptic parameters, which (as force constants) reflect peculiarities of electron density distribution of molecules, but also to build theoretical IR-spectra of studied molecules, what allow directly visually to compare theoretically received spectra with their experimental IR-spectra. The frequency task has been earlier solved by us for the o-tolunitrile molecule. Frequencies and forms of standard vibrations of the model o-tolunitrile molecule have been calculated and the complete theoretical interpretation of its oscillatory spectrum has been carried out on forms of standard vibrations and the distribution of the potential energy on oscillatory coordinates [3]. The experimental IR-spectrum of the o-tolunitrile molecule was taken from the Saddler atlas [4].

The absorption bands intensity of IR-spectra of molecules is calculated on the base of the semiempiric theory and therefore the electrooptic parameters of molecules (dipole moments of bonds and their derivatives on oscillatory coordinates) are necessary to introduce in computer for the solution of the direct electrooptic task, when intensities and polarizations of the absorption band are calculated on the base of known electrooptic parameters. On the other hand these parameters may be calculated from experimental absorption bands of IR-spectra of molecules. It is a reverse electrooptic task, when electrooptic parameters of molecules are determined on the base of absolute intensities from the experimental spectrum. The calculated o-tolunitrile molecule model is shown on the fig.1.
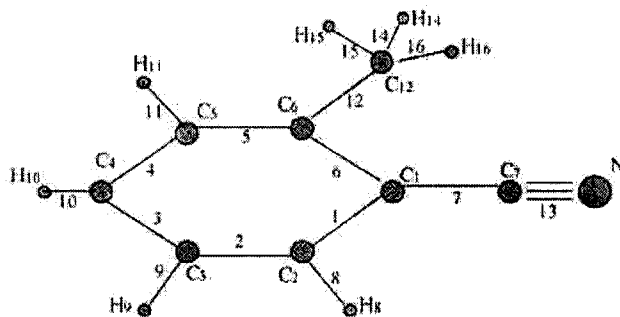

Fig.1. The calculated model and numeration of atoms and o-tolunitrile molecule bonds

The calculation was made by means of solution of direct and reverse electrooptic tasks for the o-tolunitrile molecule. The direct electrooptic task always must be solved before solving the reverse electrooptic task. If the studied molecule consists of already known fragments, then the same initial values of electrooptic parameters are given as for fragments. Initial values of electrooptic parameters for the o-tolunitrile molecule were taken from benzonitrile and ethane molecules. Theoretical values of intensities, calculated with these electrooptic parameters, for the model o-tolunitrile molecules strongly diverged from values of intensities of appropriate absorption bands of the experimental spectrum. Therefore, it is necessary to solve the reverse electrooptic task for this molecule for correction of electrooptic parameters. The parameter of calculated square difference sum and experimental intensities should be minimal at the solution of the reverse electrooptic task. Moreover, variated parameters should be in limits of the fixed interval. The interval is fixed usually on the base of additional physical considerations. The practice of solution of reverse electrooptic tasks has shown, that the choice of the change interval excludes numerous solutions of the nonlinear task.

The absolute intensity has been calculated by us for all observed absorption bands of the experimental spectrum of the o-tolunitrile molecule (see table 3) before solving of

reverse electrooptic tasks and the dependence has been analyzed of absorption bands intensities on electrooptic parameters of concrete polar bonds of the studied molecule.

Electrooptic tasks had been solved at three stages. At the first stage the electrooptic task had been solved for dipole moments of bonds of the o-tolunitrile molecule. Values of dipole moments had been variated before achievement of the best conformity of theoretical and experimental values of intensities of those absorption bands, which depend on these dipole moments. Values of dipole moments, calculated after solving of the reverse electrooptic task, are shown in the table 1, where initial values of dipole moments are pointed in brackets.

Table 1

Dipole moments of bonds of the o-tolunitrile molecule

μ_7=0.390(-0.427)	μ_8=0.844(0.816)	μ_9=0.844(0.816)	μ_{10}=0.288(0.480)
μ_{11}=0.844(0.816)	μ_{12}=-0.593(-0.13)	μ_{13}=1.602(2.020)	μ_{14}=0.101(0.305)
μ_{15}=0.101(0.305)	μ_{16}=0.101(0.315)		

At second and third stages, reverse electrooptic tasks had been solved by us for dipole moments derivatives on oscillatory coordinates, correspondingly, for non-plane and plane vibrations of the o-tolunitrile molecule and calculated values of electrooptic parameters are shown in the table 2.

Table 2.

Derivatives of dipole moments of bonds of the o-tolunitrile molecule on its oscillatory coordinates.

$\dfrac{\partial\mu_7}{\partial\theta_1}=-0.026\,(0.041)$	$\dfrac{\partial\mu_7}{\partial\theta_7}=-2.275\,(-2.263)$	$\dfrac{\partial\mu_7}{\partial\theta_{19}}=-0.610\,(0.557)$
$\dfrac{\partial\mu_7}{\partial\theta_{21}}=0.495\,(0.451)$	$\dfrac{\partial\mu_7}{\partial\theta_{30}}=-0.041\,(-0.030)$	$\dfrac{\partial\mu_7}{\partial\theta_{43}}=0.560\,(0.560)$
$\dfrac{\partial\mu_7}{\partial\theta_{44}}=-0.578\,(-0.451)$	$\dfrac{\partial\mu_8}{\partial\theta_1}=-0.014\,(-0.019)$	$\dfrac{\partial\mu_8}{\partial\theta_8}=0.470\,(0.490)$
$\dfrac{\partial\mu_8}{\partial\theta_{20}}=-0.813\,(-0.203)$	$\dfrac{\partial\mu_9}{\partial\theta_{22}}=0.001\,(-0.74)$	$\dfrac{\partial\mu_{11}}{\partial\theta_{29}}=-0.265\,(0.246)$
$\dfrac{\partial\mu_{12}}{\partial\theta_5}=0.173\,(0.392)$	$\dfrac{\partial\mu_{12}}{\partial\theta_{12}}=-0.425\,(-0.477)$	$\dfrac{\partial\mu_{12}}{\partial\theta_{18}}=-0.280\,(0.610)$
$\dfrac{\partial\mu_{12}}{\partial\theta_{19}}=-0.302\,(-0.317)$	$\dfrac{\partial\mu_{12}}{\partial\theta_{28}}=0.551\,(0.260)$	$\dfrac{\partial\mu_{12}}{\partial\theta_{29}}=0.033\,(0.432)$
$\dfrac{\partial\mu_{12}}{\partial\theta_{45}}=-0.111\,(-0.138)$	$\dfrac{\partial\mu_{12}}{\partial\theta_{48}}=-0.190\,(-0.270)$	$\dfrac{\partial\mu_{12}}{\partial\theta_{51}}=0.352\,(0.491)$
$\dfrac{\partial\mu_{13}}{\partial\theta_7}=-0.128\,(-0.116)$	$\dfrac{\partial\mu_{13}}{\partial\theta_{19}}=-0.032\,(0.022)$	$\dfrac{\partial\mu_{13}}{\partial\theta_{43}}=-0.203\,(-0.230)$
$\dfrac{\partial\mu_{13}}{\partial\theta_{44}}=-0.571\,(0.750)$	$\dfrac{\partial\mu_{14}}{\partial\theta_{45}}=0.439\,(0.476)$	$\dfrac{\partial\mu_{14}}{\partial\theta_{46}}=-0.151\,(0.126)$

Results of the theoretical calculation of the oscillatory spectrum intensities of the o-tolunitrile molecule are shown in the table 3, where calculated values of theoretical intensities and their comparison with experimental values of intensities are shown for each observed experimental band, and also values of contributions of all electrooptic parameters, taking part in creation of all absorption bands of the IR-spectrum of the o-tolunitrile molecule, are shown.

Absorption bands of the o-tolunitrile molecule may be divided on 4 groups, taking into account the analysis of theoretically calculated values for electrooptic parameters of the o-tolunitrile molecule and dependences of absorption bands intensities of the IR-spectrum of the o-tolunitrile molecule on these parameters.

The intensity of bands of the first group depends on different combinations of dipole moments of polar bonds and on dipole moments derivatives on oscillatory coordinates of the structural element C-C=N. These absorption bands are observed in the low-frequency region of the spectrum: 430, 342, 566, 706, and 1006 cm^{-1}.

The second group of bands is absorption bands 962, 987, 1047, 1455, 2919 and 2920 cm^{-1}, whose intensity depends on dipole moments of CH bonds of benzene ring and dipole moments of CH bonds of CH$_3$ group. Moreover, the intensity of these absorption bands depends also on dipole moments derivatives of CH bonds, coming into the C-CH$_3$ group. The band at 1455 cm^{-1} is the most intensive band among these absorption bands.

The third group. Absorption bands intensity of this spectrum region depends on dipole moments of all polar CH bonds and their derivatives on angle oscillatory coordinates. Moreover intensities of some these bands depend also on dipole moments of the C-C=N group.

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Table 3.

Experimental and theoretical frequencies and absorption bands intensities of the IR-spectrum of the o-tolunitrile molecule.

$V_{exper.}$	$I_{exper.}$	$I_{theor.}$	Contribution, μ	Dipole moments	Contribution $\partial\mu_i/\partial\theta_j$	Derivatives of dip.mom. on oscil.coord.
3069	5.70	4.3			0.377	$\partial\mu_8/\partial q_8$
3063	9.79	9.5			-0.593	$\partial\mu_8/\partial q_8$
30589	1.87				0.393 0.066	$\partial\mu_8/\partial q_8$ $\partial\mu_8/\partial q_{23}$
3057	0.12	0.3			-0.08	$\partial\mu_8/\partial q_8$
2920	3.19	3.0	-0.076 0.051	$\mu_8,\ \mu_9,\ \mu_{11},\ \mu_{12}$	-0.611 -0.610	$\partial\mu_8/\partial q_{46}$ $\partial\mu_8/\partial q_{45}$
2919	3.54	3.2	0.087 -0.059	$\mu_{14},\ \mu_{14},\ \mu_{16},\ \mu_{12}$	1.221 -1.221 -0.123 0.123 0.102 -0.102	$\partial\mu_{14}/\partial q_{45}$ $\partial\mu_{14}/\partial q_{46}$ $\partial\mu_{14}/\partial q_{48}$ $\partial\mu_{14}/\partial q_{49}$ $\partial\mu_{14}/\partial q_{51}$ $\partial\mu_{14}/\partial q_{52}$
2849	1.13	1.01	0.061	$\mu_{14},\ \mu_{15},\ \mu_{16}$	1.521 1.014 0.507 0.071	$\partial\mu_8/\partial q_8$ $\partial\mu_8/\partial q_8$ $\partial\mu_8/\partial q_8$ $\partial\mu_8/\partial q_8$
2233	10.72	9.3			0.407 0.407 -0.271 -0.271	$\partial\mu_7/\partial q_{43}$ $\partial\mu_{13}/\partial q_{43}$ $\partial\mu_{13}/\partial q_7$ $\partial\mu_7/\partial q_7$
1618	1.77	1.0		$\mu_{14},\ \mu_{15},\ \mu_{16}$ μ_7 μ_{10}	0.373 -0.311 0.281 -0.279 0.279 -0.244 -0.128 -0.115	$\partial\mu_8/\partial q_{23}$ $\partial\mu_2/\partial q_{28}$ $\partial\mu_{12}/\partial q_5$ $\partial\mu_{12}/\partial q_{18}$ $\partial\mu_{12}/\partial q_{29}$ $\partial\mu_{12}/\partial q_{19}$ $\partial\mu_{12}/\partial q_{19}$ $\partial\mu_{14}/\partial q_{49}$
1610	2.56	1.8	0.115 -0.104 0.084	$\mu_8,\ \mu_9,\ \mu_{11},$ μ_{10} μ_7	-0.211 0.205 -0.189 0.154 0.143 0.110 -0.108	$\partial\mu_8/\partial q_{20}$ $\partial\mu_{11}/\partial q_{29}$ $\partial\mu_{14}/\partial q_{48}$ $\partial\mu_{14}/\partial q_{49}$ $\partial\mu_{14}/\partial q_{52}$ $\partial\mu_{12}/\partial q_5$ $\partial\mu_{14}/\partial q_{51}$
1492	8.03	3.3		$\mu_8,\ \mu_9,\ \mu_{11}$ μ_{10} $\mu_{14},\ \mu_{15},\ \mu_{16}$	-0.913 -0.452 0.266 0.204 -0.186 0.166	$\partial\mu_8/\partial q_{23}$ $\partial\mu_{12}/\partial q_{28}$ $\partial\mu_8/\partial q_1$ $\partial\mu_{12}/\partial q_{48}$ $\partial\mu_{12}/\partial q_{51}$ $\partial\mu_{12}/\partial q_{52}$
1455	2.49	2.2	-0.794	$\mu_{14}, \mu_{15}, \mu_{16}$	-1.823 1.823 -0.573 0.573	$\partial\mu_{14}/\partial q_{51}$ $\partial\mu_{14}/\partial q_{52}$ $\partial\mu_{14}/\partial q_{48}$ $\partial\mu_{14}/\partial q_{49}$
1454	6.88	5.5	0.304 0.141 0.102	$\mu_{14},\ \mu_{15},\ \mu_{16}$ μ_{10} μ_8, μ_9, μ_{11}	0.868 -0.794 -0.515 -0.311 0.238 0.198	$\partial\mu_{14}/\partial q_{51}$ $\partial\mu_{14}/\partial q_{52}$ $\partial\mu_8/\partial q_{23}$ $\partial\mu_{14}/\partial q_{49}$ $\partial\mu_{14}/\partial q_{48}$ $\partial\mu_{12}/\partial q_{48}$
1434	4.58	4.1	-0.472 0.293 -0.186	μ_{10} $\mu_{14},\ \mu_{15},\ \mu_{16}$ μ_8, μ_9, μ_{11}	1.388 -0.470 -0.411 0.251 0.158 -0.159	$\partial\mu_8/\partial q_{23}$ $\partial\mu_8/\partial q_1$ $\partial\mu_{14}/\partial q_{52}$ $\partial\mu_{14}/\partial q_{51}$ $\partial\mu_{12}/\partial q_{18}$ $\partial\mu_{12}/\partial q_{19}$

1378	4.44	3.9	-1.365 -0.158 -0.140	$\mu_{14}, \mu_{15}, \mu_{16}$ μ_{10} μ_8, μ_9, μ_{11}	-1.565 1.565 1.061 -1.048 -0.517 0.504 0.432	$\partial\mu_{12}/\partial q_{48}$ $\partial\mu_{12}/\partial q_{51}$ $\partial\mu_{14}/\partial q_{52}$ $\partial\mu_{14}/\partial q_{49}$ $\partial\mu_{14}/\partial q_{48}$ $\partial\mu_8/\partial q_{23}$ $\partial\mu_{12}/\partial q_{28}$
1300	1.01	0.8	0.126 -0.074 0.058	μ_8, μ_9, μ_{11} $\mu_{14}, \mu_{15}, \mu_{16}$ μ_7	0.224 -0.220 0.220 -0.171 -0.148	$\partial\mu_{14}/\partial q_{51}$ $\partial\mu_{12}/\partial q_{48}$ $\partial\mu_{12}/\partial q_{51}$ $\partial\mu_{14}/\partial q_{48}$ $\partial\mu_{12}/\partial q_{12}$
1283	0.75	0.9	0.292 -0.270 -0.207	$\mu_{14}, \mu_{15}, \mu_{16}$ μ_{10} μ_8, μ_9, μ_{11}	0.455 0.371 -0.371 0.313 -0.266 0.211 0.207	$\partial\mu_{12}/\partial q_{28}$ $\partial\mu_{12}/\partial q_{48}$ $\partial\mu_{12}/\partial q_{21}$ $\partial\mu_8/\partial q_{23}$ $\partial\mu_8/\partial q_1$ $\partial\mu_{14}/\partial q_{49}$ $\partial\mu_{12}/\partial q_{12}$
1251	4.465	3.8	-0.287 0.160 0.149 0.069	$\mu_{14}, \mu_{15}, \mu_{16}$ μ_8, μ_9, μ_{11} μ_{10} μ_7	-0.789 0.287 -0.234 0.234 -0.232 0.216 0.196	$\partial\mu_{18}/\partial q_{23}$ $\partial\mu_{12}/\partial q_{28}$ $\partial\mu_{12}/\partial q_{48}$ $\partial\mu_{12}/\partial q_{51}$ $\partial\mu_{14}/\partial q_{52}$ $\partial\mu_8/\partial q_1$ $\partial\mu_{12}/\partial q_{12}$
1203	1.39	0.9	0.078	$\mu_{14}, \mu_{15}, \mu_{16}$	-0.340 0.306 0.166 -0.166 -0.140 0.133	$\partial\mu_{12}/\partial q_{28}$ $\partial\mu_8/\partial q_{23}$ $\partial\mu_{12}/\partial q_{19}$ $\partial\mu_{12}/\partial q_{18}$ $\partial\mu_{12}/\partial q_5$ $\partial\mu_8/\partial q_1$
1147	0.52	0.4	-0.596 0.585 0.084	μ_8, μ_9, μ_{11} μ_{10} $\mu_{14}, \mu_{15}, \mu_{16}$	0.370 -0.343 0.097 -0.088 -0.088	$\partial\mu_{12}/\partial q_{28}$ $\partial\mu_8/\partial q_{23}$ $\partial\mu_{14}/\partial q_{49}$ $\partial\mu_{14}/\partial q_{48}$ $\partial\mu_{14}/\partial q_{52}$
1104	1.98	1.0	0.221 0.215 0.190	μ_8, μ_9, μ_{11} μ_{10} $\mu_{14}, \mu_{15}, \mu_{16}$	-0.904 -0.404 0.277 -0.201 0.182 0.175	$\partial\mu_{14}/\partial q_{51}$ $\partial\mu_{14}/\partial q_{52}$ $\partial\mu_8/\partial q_{23}$ $\partial\mu_{14}/\partial q_{49}$ $\partial\mu_{14}/\partial q_{48}$ $\partial\mu_{12}/\partial q_{48}$
1047	3.63	3.2	-0.936 0.143 -0.069	$\mu_{14}, \mu_{15}, \mu_{16}$ μ_{12} μ_8, μ_9, μ_{11}	1.117 -0.117 -0.546 0.546	$\partial\mu_{14}/\partial q_{48}$ $\partial\mu_{14}/\partial q_{49}$ $\partial\mu_{14}/\partial q_{51}$ $\partial\mu_{14}/\partial q_{52}$
1027	4.42	3.6	-0.183 0.171 -0.170	μ_8, μ_9, μ_{11} $\mu_{14}, \mu_{15}, \mu_{16}$ μ_{10}	0.372 0.360 -0.215 0.206 0.172 -0.101	$\partial\mu_8/\partial q_1$ $\partial\mu_8/\partial q_{53}$ $\partial\mu_8/\partial q_{48}$ $\partial\mu_{14}/\partial q_{49}$ $\partial\mu_{12}/\partial q_{28}$ $\partial\mu_8/\partial q_{20}$
1006	2.71	2.1	0.566 -0.565 0.056	μ_8, μ_9, μ_{11} μ_{10} $\mu_{14}, \mu_{15}, \mu_{16}$	-0.065 0.065	$\partial\mu_{14}/\partial q_{48}$ $\partial\mu_{14}/\partial q_{49}$
987	0.50	0.3	0.0638 0.083 -0.248	$\mu_{14}, \mu_{15}, \mu_{16}$ μ_{10} μ_8, μ_9, μ_{11}	-0.419 0.419 0.180 -0.180 0.075	$\partial\mu_{14}/\partial q_{49}$ $\partial\mu_{14}/\partial q_{48}$ $\partial\mu_{14}/\partial q_{52}$ $\partial\mu_{14}/\partial q_{51}$ $\partial\mu_8/\partial q_1$
962	4.39	2.3	0.717	μ_8, μ_9, μ_{11}	0.094	$\partial\mu_{14}/\partial q_{48}$

			-0.374 -0.086	μ_{10} $\mu_{14}, \mu_{15}, \mu_{16}$	-0.094	$\partial\mu_{14}/\partial q_{49}$
871	0.64	0.7	-0.282	μ_{10}		
814	0.77	0.5	-0.095 -0.088 0.055	$\mu_{14}, \mu_{15}, \mu_{16}$ μ_{10} μ_7	0.209 0.126 0.119 0.098 -0.085	$\partial\mu_8/\partial q_{23}$ $\partial\mu_7/\partial q_{21}$ $\partial\mu_{12}/\partial q_{12}$ $\partial\mu_{12}/\partial q_5$ $\partial\mu_8/\partial q_1$
756	19.12	17.2	1.129 0.505 -0.095	μ_8, μ_9, μ_{11} μ_{10} μ_7	0.136 0.136	$\partial\mu_7/\partial q_{44}$ $\partial\mu_{13}/\partial q_{44}$
715	6.19	6.0	0.486 0.285 -0.104 0.100	μ_8, μ_9, μ_{11} μ_{10} $\mu_{14}, \mu_{15}, \mu_{16}$ μ_7	-0.133 -0.133 0.074 -0.074	$\partial\mu_7/\partial q_{44}$ $\partial\mu_{13}/\partial q_{44}$ $\partial\mu_{14}/\partial q_{48}$ $\partial\mu_{14}/\partial q_{29}$
706	1.62	0.9	0.151 -0.070 0.056	μ_8, μ_9, μ_{11} $\mu_{14}, \mu_{15}, \mu_{16}$ μ_{10}	-0.108 -0.105 -0.148 0.118 0.118 -0.111 -0.111	$\partial\mu_{12}/\partial q_{28}$ $\partial\mu_{12}/\partial q_5$ $\partial\mu_7/\partial q_1$ $\partial\mu_7/\partial q_{19}$ $\partial\mu_{13}/\partial q_7$ $\partial\mu_7/\partial q_7$ $\partial\mu_7/\partial q_{21}$
566	7.8	6.1	-0.472 -0.193 0.105 0.105	μ_8, μ_9, μ_{11} μ_7 μ_{10} μ_{13}	0.321 0.325	$\partial\mu_7/\partial q_{44}$ $\partial\mu_{13}/\partial q_{44}$
535	1.45	1.1	-0.070 0.059 -0.056	μ_{10} μ_{13} μ_7	0.149 -0.149 0.113 0.110	$\partial\mu_{12}/\partial q_{18}$ $\partial\mu_{12}/\partial q_{29}$ $\partial\mu_8/\partial q_{20}$ $\partial\mu_{12}/\partial q_{19}$ $\partial\mu_8/\partial q_{23}$
461	4.98	5.5	-0.146	μ_7 μ_{13} $\mu_{14}, \mu_{15}, \mu_{16}$	0.201 0.128 0.118 -0.163	$\partial\mu_{12}/\partial q_{19}$ $\partial\mu_{11}/\partial q_{19}$ $\partial\mu_8/\partial q_{20}$ $\partial\mu_7/\partial q_{30}$
430	0.082	1.2	0.232 0.105 0.080	μ_8, μ_9, μ_{11} $\mu_{14}, \mu_1, \mu_{16}$ μ_{12}	0.097 0.097	$\partial\mu_7/\partial q_{44}$ $\partial\mu_{13}/\partial q_{44}$
401	4.77	4.0	-0.110 0.102	μ_7 μ_{13}	0.166 -0.111 0.111 -0.135 -0.135	$\partial\mu_8/\partial q_{20}$ $\partial\mu_2/\partial q_{18}$ $\partial\mu_{12}/\partial q_{19}$ $\partial\mu_7/\partial q_{19}$ $\partial\mu_{13}/\partial q_{19}$
342	4.98	3.0	-0.261 0.146 0.124	μ_{13} μ_7 μ_{10}	-0.443 -0.443	$\partial\mu_{14}/\partial q_{51}$ $\partial\mu_{14}/\partial q_{52}$

Bands with frequencies 2233, 3057, 3063 and 3069 cm⁻¹ are observed in the high-frequency region. It is the fourth group of absorption bands. The absorption bands intensity of this spectrum region does not depend on dipole moments of polar bonds. The observed absorption bands intensity of this region mainly depends on derivatives of dipole moments on oscillatory coordinates of the polar bond of the C_2H_8 type. The intensity of the absorption band 2233 cm⁻¹ is determined by the derivative of the dipole moment of the C-C=N group on oscillatory coordinates. It has been established by means of the theoretical study, that bands 566, 756, 871, 962, 1006, 1455, 1919, 1920 and 3057cm⁻¹ are completely polarized. Bands 756, 871, 962 and 1006 cm⁻¹ display from these absorption bands at the expense of the vibration of bond exit type from the plane.

The theoretical IR-spectrum, which has been visually compared with the experimental spectrum of this molecule, has been built by us with calculated values of electrooptic parameters after solving of the reverse electrooptic task of the _o_-tolunitrile molecule. The comparison of these spectral curves shows, that the received theoretical curve of the spectral distribution of the absorption coefficient describes quite satisfactory the experimental spectrum of the _o_-tolunitrile molecule, that proves the reliability of determined by us electrooptic parameters of this molecule.
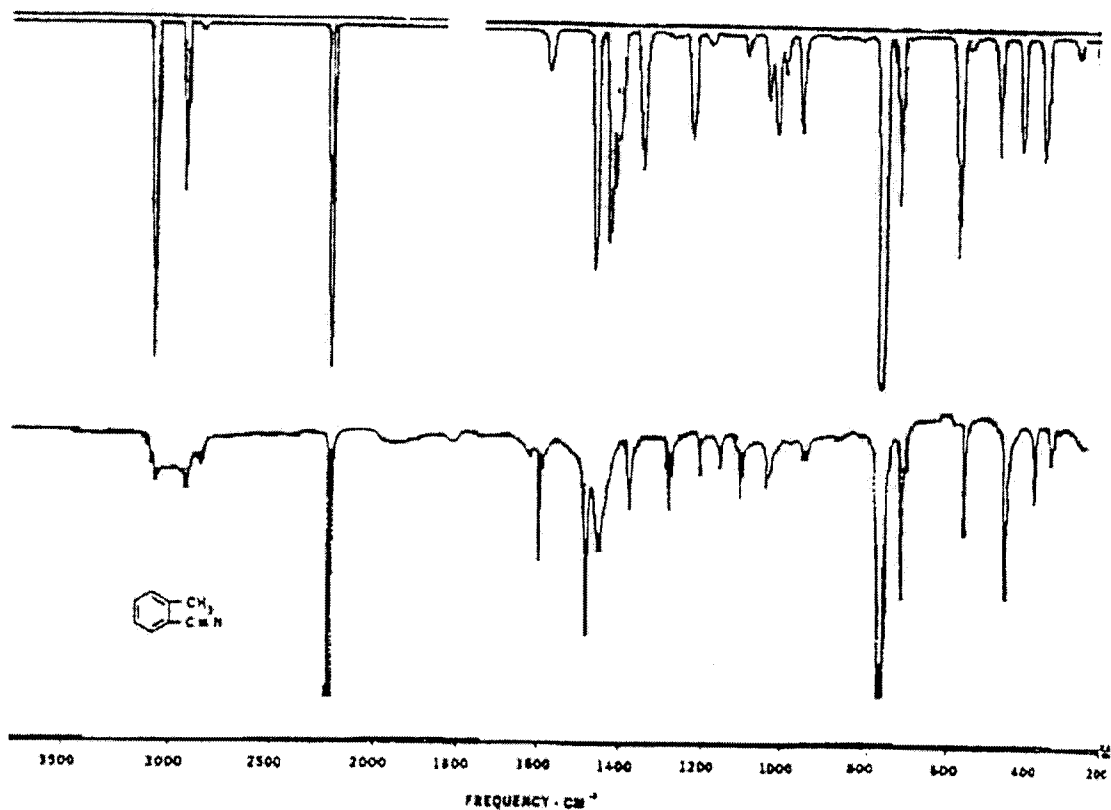
Fig. 2 The theoretical (upper) and experimental spectrum of the *o*-tolunitrile molecule.

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O-TOLUNİTRİL MOLEKULUNUN İQ SPEKTRİNİN UDMA ZOLAQLARININ İNTENSİVLİYİNİN HESABLANMASI

Nəzəri rəqs spectroskopiyası metodu ilə *o*-tolunitril molekulunun İQ spektrinin udma zolaqlarının intensivliyi tədqiq olunmuş-dur. Molekulunun İQ-spektrinin udma zolaqlarının intensivliyinin nəzəri qiymətləri təyin olunmuşdur. Elektrooptik parametrlər toplusu tapılmış və udma zolaqlarının təbiəti təhlil edilmişdir. Udma əmsalının spektrdə paylanması əyrisi qurulmuşdur.

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РАСЧЕТ ИНТЕНСИВНОСТЕЙ ПОЛОС ПОГЛОЩЕНИЯ ИК-СПЕКТРА МОЛЕКУЛЫ O-ТОЛУНИТРИЛ

Методом теоретической колебательной спектроскопии произведено теоретическое исследование интенсивностей полос поглощения ИК спектра молекулы *o*-толунитрил. Получены теоретические значения интенсивностей полос поглощения ИК-спектра молекулы, найден набор электрических параметров, проведен анализ природы появления каждой полосы поглощения и построена теоретическая кривая спектрального распределения коэффициента поглощения молекулы *o*-толунитрил.