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The methods of optical physics as a mean of the objects’ molecular structure identification (on the base of the research of dophamine and adrenaline molecules)

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Abstract. Structural and dynamic models of dopamine and adrenaline are proposed on the basis of ab initio quantum calculations of the geometric and electronic structure. The parameters of the adiabatic potential are determined, a vibrational states interpretation of the test compound is proposed in this work. The analysis of the molecules conformational structure of the substance is made. A method for calculating the shifts of vibrational excitation frequencies in 1,2,4-threesubstituted of benzole is presented. It is based on second order perturbation theory. A choice of method and basis for calculation of a fundamental vibrations frequencies and intensities of the bands in the IR and Raman spectra is justified. The technique for evaluation of anharmonicity with cubic and quartic force constants is described. The paper presents the results of numerical experiments, geometric parameters of molecules, such as the valence bond lengths and angles between them. We obtain the frequency of the vibrational states and values of their integrated intensities. The interpretation of vibration of conformers is given. The results are in good agreement with experimental values. Proposed frequency can be used to identify the compounds of the vibrational spectra of molecules. The calculation was performed quantum density functional method DFT/B3LYP. It is shown that this method can be used to modeling the geometrical parameters molecular and electronic structure of various substituted of benzole. It allows us to construct the structural-dynamic models of this class of compounds by numerical calculations.

1. Introduction
Detecting the features of compounds spectral identification, their interpretation or their relation to a certain molecular fragment are both fundamental target of mathematical modeling in the theory of molecular system and applied one according to the quantitative and qualitative composition of bioobjects i.e. relations “State-Structure- Spectrum”. The achievement of the given problem possesses its own special features for each composition. The present work demonstrates the possibility of the use of the up-to-date programming software to create structural and dynamical models of the substance and accomplishment on the base of the spectrum identification of the substance. Optical physics methods are the most informative in the studied structures of the discussed types of the molecular objects.

Solving problems of the discussed types is possible due to the high techs of the molecular modeling i.e. the use of quantum method of analyses of parameters of adiabetic potential. These methods in the beginning of the 21 century completely replaced the classical methods of molecular dynamics which are based on the soluteon of inverse problems in theoretical physics. The applied methods are imple-
mented as applied programming lay-outs. Dominating one is “Gaussian” according to the frequency use. Its particular feature is the implementation of the method of functional density DFT/B3LYP allowing to model effectively the problems discussed in article.

The interest to the study of the structure and spectrum of molecule of dopamine and adrenaline is understandable (Figure 1). As an example we refer to the works [1,2,3] where just one of the possible conformers’ combinations. Interesse к изучению структуры и спектра молекул дофамина и адреналина (рис.1) понятен. Сошлемся, к примеру, на работы [1,2,3], где рассмотрен лишь один (A) из возможных конформеров соединений. In the work [3] such interpretation for high frequency range is differ from data given in study [4]. In the work [1] there used a classical approach to evaluate the parameters of harmonic force field. In the work [2] the authors researched the range of 570-1880 sm⁻¹. The spectrum modeling calculation are limited by harmonic approximation of the molecular vibrations theory. To measure anharmonic displacement there used the procedure of scaling [5].

Structurally dopamine and adrenaline are related to 1,2,4 – benzol substituents(C₆H₃XYZ).According to the study[6] the number of fundamental vibrations of benzol trisubstitution could be divided into following groups: characterized by frequency,mode and intensity, characterized by frequency and mode, characterized by mode. Theoretical interpretation of fundamental vibrations of spectrum suggested in the work [6] completely agrees with experimental fundamental vibrations spectrum allocation 1,2,4 – benzol substituted (X=F, CH₃), suggested in the work [7]. This gives the possibility to assume that the given interpretation of spectrum skeleton will possess a space for both dopamine molecules and (X,Y=OH, Z=CH(NH₂) and adrenaline (X,Y=OH, Z=CH(NH₂). The accuracy of such idea could be confirmed by quantum calculations.

The given work suggests structural and dynamical models of possible dopamine and adrenaline conformers on the base of model quantum calculations. All calculations are carried out according to the density functional method DFT/B3LYP [8] with the use of the basis 6-311G*, 6-311G**, 6-311+G**.

2. Methods
The evaluation of the bands’ state was carried out by means of the following ratio [9]

\[ E_v = v + \frac{1}{2} + \chi_{sr} (n_x + 1/2) (n_y + 1/2) \]  

There used the equation from the work [10] for anharmonic constants \( \chi_{sr} \).
\[
\chi_{ss} = \frac{1}{16} F_{ss} - \frac{5}{48} \left( \frac{F_{s1}}{v_s} \right)^2 + \frac{1}{32} \left( \frac{F_{s2}}{v_s} \right)^2 \left( \Omega(s; s, r) - \Omega(s; s, r) - 12 \Omega(r, r, r) \right) (1 - \delta_{ss})
\]

\[
\chi_{tt} = \frac{1}{16} F_{tt} - \frac{1}{8} \left( \frac{F_{e1}}{v_e} \right)^2 \left( \Omega(s; s; r) + \Omega(s; s; r) (1 - \delta_{ss}) \right) + \frac{3}{8} \left( \frac{F_{e2}}{v_e} \right)^2 \left( \Omega(s; r; t) - \Omega(s; r; t) - \Omega(s; t; t) \right) \times
\]

\[
(1 - \delta_{ss}) (1 - \delta_{tt}) (1 - \delta_{tt}) + L(a; sr) \cdot P_r \cdot L(a; st)
\]

\[
\Omega(s; s, r) = \frac{1}{2} \Omega(s; s, r) + \Omega(s; s, r) + \Omega(s; r, r) - \Omega(s; r, r) - \Omega(s; t, t) - \Omega(s; t, t) - \Omega(s; t, t) - \Omega(s; r, t) - \Omega(r, r, r)
\]

Here \( P_r = L(a; sr) Q^2 \cdot P_r \cdot L(a, st) \) – constants Coriolis, \( v_s, v_e \) – harmonic vibrations frequency (in sm\(^{-1}\)); \( Q^2 \) – dimensionless normal vibration coordinates; \( F_{sr}, F_{sr1} \) – cubic and quatic force constants, \( \Omega(s; s, r) \) – resonance functions, \( n_i \) – the quantum number of vibration state.

When testing the method DFT/B3LYP resources, during the primarily calculations of geometrical and electronic structures 1,2,4-trisubstituted benzol, there used relevant difluoro and dihydroxytoluene. The given approach was used in the works [11-12] when constructing structural and dynamical models of a number of trisubstituted benzol.

3. Results

According to the calculations the geometrical structure of benzol ring when being replaced is not changed greatly. The length of the valence bonds are distinguished by the amount of \( ~0.008 \) Å, values of the bond angles \( ~1.6^\circ \).

The results of model calculations of the vibrational state of the benzol skeleton of the possible conformers of the given test compositions completely agree with the experimental fundamental frequency assignment suggested in the works [1,6,7].

In studied conformers of 1,2-dihydro-4-methyl benzol, the great interest is in the band position which are interpreted as valent \( q_{OH} \) and non-plane deformational vibrations \( q_{OH} \) of hydroxyl sections. These are the doublets \( ~3710 \) and \( 3650 \text{ sm}^{-1} \) in highly frequency range of vibrational spectrum for conformers A and B. The bands are identical for the third conformer \( ~3700 \text{ sm}^{-1} \). We can notice that in the works [1,3] the value of frequency being interpreted as valent frequency bonds OH \( q_{OH} \) is transformed into long waved area of the frequency spectrum for \( ~300 \text{ sm}^{-1} \) in comparison with data given above and suggested assignment for the mentioned frequency from the work [8]. Due to the fact that the relevant experiment introduced in the works [1,3] corresponds to the condensing state of dopamine and adrenaline.

The band state interpreted as torsion vibrations \( q_{OH} \), is characterized by the following doublets: 410 and \( 210 \text{ sm}^{-1} \), 420 and \( 170 \text{ sm}^{-1} \), 360 and \( 310 \text{ sm}^{-1} \). According to the model calculations the bands are the most intensive in a low frequency range of vibrational spectrum.

The most important fact is the vibrational characteristics of the benzol skeleton according to the frequency. There can be observed characteristics according to the intensity for the given type of benzol trisodium while interfusing according to the form for deformational vibrations of hydroxide fragments. The testing results confirm the suggested theory. The intensity band changing values is connected either with the varied electronic substitutes’ properties or with the interfusion of ordinary vibrations forms interpreted as deformational vibrations of the relations CH (H=H, F, O) in the model calculations. It can be seen in 1,2 dihydro- 4 methyl benzol in the range of ~ 1550-1100 sm\(^{-1}\).

The interpretation of vibrational spectrum of dopamine is introduced in the table 1. It was supposed that a molecule belongs to the symmetry group \( C_2 \) (the carboatomic plane is the molecule symmetry plane). Torsional vibrations were produced when the fragments \( \text{CH}_3\text{C} \) and \( \text{CH}_2\text{NH}_2 \) of substitutes are in the transconfiguration relatively each other.
| Form of vibration | $v_{\text{measured}}$ [cm$^{-1}$] | $v_{\text{r}}$ | Model_A | Model_B | Model_C |
|------------------|---------------------------------|-------------|----------|----------|----------|
|                  | $v_{\text{aur}}$ | IR | CR | $v_{\text{aur}}$ | IR | CR | $v_{\text{aur}}$ | IR | CR |
| Flat vibrations of 1,2,4 trisubstituted benzol fragment фрагметта (symmetry A') | | | | | | | | | |
| $Q,\gamma,\beta$ | 1621 | 1663 | 1621 | 9.6 | 37 | 1622 | 20 | 8.7 | 1618 | 4.1 | 32 |
| $\rho$ | 1596 | 1645 | 1605 | 178 | 6.1 | 1601 | 39 | 8.5 | 1601 | 35 | 12 |
| $\beta,Q$ | 1522 | 1559 | 1521 | 146 | 2.0 | 1511 | 188 | 1.1 | 1526 | 138 | 1.5 |
| $\beta_{\text{OH}},\beta$ | 1382 | 1404 | 1376 | 38 | 6.7 | 1369 | 6.2 | 3.7 | 1364 | 14 | 5.1 |
| $\beta_{\text{OH},\beta}$ | 1326 | 1354 | 1319 | 13 | 1.0 | 1321 | 140 | 1.9 | 1324 | 7.6 | 1.2 |
| $Q_{\text{CO}},Q$ | 1277 | 1314 | 1279 | 114 | 13 | 1281 | 126 | 13 | 1286 | 104 | 11 |
| $Q_{\text{CO},\beta_{\text{OH}}}$ | 1234 | 1292 | 1259 | 132 | 1.1 | 1256 | 48 | 0.6 | 1266 | 30 | 2.6 |
| $\beta_{\text{OH},\beta}$ | 1188 | 1214 | 1193 | 54 | 8.3 | 1188 | 31 | 5.3 | 1174 | 309 | 1.0 |
| $\beta_{\text{OH},\beta}$ | 1176 | 1185 | 1149 | 75 | 3.4 | 1153 | 102 | 4.1 | 1169 | 67 | 3.2 |
| $\gamma,\beta_{\text{OH}}$ | 1099 | 1128 | 1103 | 107 | 1.0 | 1101 | 92 | 4.3 | 1100 | 82 | 1.3 |
| $\gamma$ | 922 | 958 | 931 | 2.7 | 5.8 | 937 | 13 | 5.0 | 939 | 12 | 4.7 |
| $\gamma$ | 771 | 794 | 779 | 39 | 18 | 775 | 48 | 18 | 774 | 22 | 18 |
| $\gamma$ | 728 | 758 | 741 | 5.8 | 8.4 | 741 | 10 | 7.3 | 742 | 7.2 | 8.7 |
| $\beta_{\text{CO},\gamma}$ | 571 | 588 | 579 | 19 | 2.8 | 578 | 9.3 | 5.4 | 567 | 10 | 3.3 |
| $\beta_{\text{CC},\beta_{\text{CC}}}$ | 445 | 467 | 456 | 3.4 | 1.0 | 456 | 5.7 | 0.9 | 460 | 4.2 | 1.5 |
| $\beta_{\text{CC},\beta_{\text{CC}}}$ | 340 | 337 | 330 | 9.5 | 0.3 | 330 | 1.0 | 0.3 | 330 | 0.6 | 0.6 |
| $\beta_{\text{CO},\gamma}$ | 312 | 316 | 310 | 3.2 | 3.6 | 309 | 6.3 | 3.3 | 310 | 16 | 2.2 |
| $\beta_{\text{CO},\gamma}$ | 285 | 297 | 291 | 2.2 | 4.9 | 292 | 3.7 | 4.3 | 290 | 1.8 | 6.1 |
| Non-flat vibrations of 1,2,4 trisubstitute fragment (symmetry A) | | | | | | | | | |
| $\rho$ | 932 | 936 | 914 | 1.6 | 0.2 | 890 | 3.5 | 0.1 | 887 | 1.0 | 0.1 |
| $\rho$ | 854 | 849 | 818 | 29 | 0.6 | 851 | 11 | 0.7 | 820 | 24 | 0.8 |
| $\rho$ | 804 | 807 | 806 | 13 | 0.7 | 780 | 29 | 0.4 | 783 | 22 | 0.7 |
| $\chi_{\rho},\rho$ | 688 | 706 | 690 | 0.1 | 0.1 | 689 | 0.2 | 0.1 | 691 | 0.2 | 0.1 |
| $\rho,\chi_{\text{CO}}$ | 603 | 600 | 584 | 9.9 | 0.3 | 588 | 4.4 | 0.1 | 588 | 7.6 | 0.2 |
| $\chi_{\text{CO},\chi}$ | 434 | 456 | 445 | 2.9 | 0.9 | 448 | 11 | 1.3 | 446 | 1.6 | 0.2 |
| $\rho_{\text{CO},\chi}$ | 330 | 343 | 350 | 7.7 | 2.2 | 352 | 4.3 | 2.5 | 306 | 6.7 | 4.8 |
| $\chi$ | 237 | 223 | 220 | 2.5 | 1.2 | 224 | 19 | 0.3 | 213 | 4.9 | 1.4 |
lecu
deformational vibration of the bond
in classical theory of molecular vibrations.
fins and methylamine [5] confirms the relevance of the harmonic strain constanta from the close m o-
firm  the arguments given above which are related to dopamine spectrum identification. All fund a-
stituted benzol allows to interpret the fundamental vibrations of the fragment of
400 sm$^{-1}$ (1200-1400 cm$^{-1}$) for the conformers compounds spectral identification.

NH2 leads to the same patterns in the frequency vibrations behavior that happen while trans-
ations the bands' position and evaluation of their intensity. The second group is interpreted as the vibr
mental vibrations of the compounds could be divided into two groups. The first one is connected with
benzol skeleton of 1,2,4- trisub-
ferred from methylamine to dimethylamine [5]. The bands interpreted as valent (q
agreem
Note: Vibrational frequency in sm$^{-1}$.Intensity in IR spectrum in km/mole , in spectrum CR Å$^{-1}$ a.e.m.

| $\chi$ | 152 | 157 | 155 | 4.7 | 1.0 | 156 | 0.1 | 0.5 | 152 | 0.1 | 0.5 |
|--------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| $q_{\text{OH}}$ | 3615 | 3844 | 3712 | 69 | 103 | 3714 | 79 | 125 | 3698 | 42 | 152 |
| $q_{\text{OH}}$ | 3803 | 3658 | 101 | 77 | 3654 | 102 | 78 | 3696 | 72 | 75 |
| $q_{\text{NH}}$ | 3427 | 3553 | 3432 | 0.1 | 60 | 3431 | 0.1 | 61 | 3431 | 0.1 | 60 |
| $q_{\text{NH}}$ | 3360 | 3478 | 3361 | 1.1 | 110 | 3360 | 1.0 | 111 | 3360 | 1.1 | 110 |
| $\gamma_{\text{NH}}$ | 1623 | 1666 | 1622 | 27 | 5.2 | 1624 | 5.0 | 24 | 1622 | 24 | 5.6 |
| $\alpha_{\text{CN}}$ | 1430 | 1388 | 1364 | 10 | 6.2 | 1349 | 8.0 | 11 | 1350 | 52 | 16 |
| $Q_{\text{CN}}$ | 1059 | 1092 | 1067 | 8.2 | 6.6 | 1067 | 3.7 | 5.4 | 1066 | 3.9 | 6.0 |
| $Q_{\text{CC}}$ | 1040 | 1049 | 1025 | 34 | 1.8 | 1024 | 74 | 2.4 | 1025 | 44 | 2.3 |
| $\beta_{\text{CN}}$ | 780 | 861 | 840 | 223 | 3.8 | 844 | 198 | 3.1 | 843 | 217 | 3.3 |
| $\chi_{\text{OH}}$ | - | - | 415 | 70 | 1.2 | 424 | 66 | 1.0 | 362 | 63 | 2.4 |
| $\chi_{\text{OH}}$ | 303 | - | 199 | 141 | 3.0 | 190 | 131 | 4.3 | 311 | 137 | 0.1 |
| $\chi_{\text{CN}}$ | - | 293 | 287 | 41 | 1.9 | 287 | 42 | 1.9 | 287 | 49 | 1.8 |

For the spectrum identification of conformers there can be used IR bands intensity in the range of 1200-1400 cm$^{-1}$ and the bands interpreted as deformational non-flat vibrations of the bonds $\text{OH}$ ($\chi_{\text{OH}}$). The use of the basis 6-311G++ [7] leads to the displacement of calculated values of vibrations ($\Delta \approx 50$ cm$^{-1}$). But the significant intensity of the given bands in IR spectrum in the range of lower than 400 sm$^{-1}$ does not create difficulties in the interpretation of low frequency range.

The determination conformity related to the spectrum bands of the benzol fragment of 1,2,4- trisub-
stituted benzol allows to interpret the fundamental vibrations of the fragment of $\text{CH}_2\text{CH}_2\text{NH}_2$. Their agreement with the experimental data on the characteristic frequency vibrations for the normal paraffins and methylamine [5] confirms the relevance of the harmonic strain constanta from the close molecular fragments system system transfer scheme used in the work of [5] to solve the reverse problems in classical theory of molecular vibrations.

The interpretation of spectrum fundamental vibrations of adrenaline suggested in the table 2 confirms the arguments given above which are related to dopamine spectrum identification. All fundamental vibrations of the compounds could be divided into two groups. The first one is connected with benzol skeleton of $\text{C}_8\text{H}_x\text{X}_y$. The adrenaline symmetry decrease to the group of $\text{C}_8$ does not influence on the bands’ position and evaluation of their intensity. The second group is interpreted as the vibrations of the fragment $\text{CHOH-CH}_2\text{NHCH}_3$. The hydrogen atom substitution into the methyl group in the fragment $\text{NH}_2$ leads to the same patterns in the frequency vibrations behavior that happen while transferring from methylamine to dimethylamine [5]. The bands interpreted as valent ($q_{\text{OH}}$) and nonplane deformatonal vibration of the bond $\text{OH}$ ($\gamma_{\text{OH}}$) of the fragment $\text{CHOH-CH}_2\text{NHCH}_3$ is difficult to use for the conformers compounds spectral identification.
| Form of vibration | Model A |  |  | Model B |  |  | Model C |  |  |
|-------------------|---------|-----|-----|---------|-----|-----|---------|-----|-----|
|                   | $\nu_{\text{arr}}$ | IR | CR | $\nu_{\text{arr}}$ | IR | CR | $\nu_{\text{arr}}$ | IR | CR |
| $Q,\gamma,\beta$  | 1616    | 16 | 80 | 1619    | 4.4 | 68 | 1615    | 11 | 62 |
| $Q,\gamma,\beta$  | 1604    | 29 | 7.7| 1602    | 43  | 7.4| 1601    | 32 | 29 |
| $\beta$           | 1517    | 118| 9.2| 1506    | 160 | 3.0| 1520    | 118| 6.4 |
| $Q,\beta,\beta_{\text{OH}}$ | 1439 | 98  | 3.7| 1454    | 11  | 15.0| 1436    | 8.7 | 5.5 |
| $\beta,\beta_{\text{OH}}$ | 1373 | 28  | 16 | 1372    | 15  | 8.5| 1364    | 20  | 27 |
| $Q,\beta$         | 1279    | 210| 21 | 1286    | 59  | 19 | 1287    | 142 | 19 |
| $Q,\beta$         | 1274    | 23 | 1.7| 1273    | 132 | 6.9| 1280    | 3.9 | 2.5 |
| $Q_{\text{CO}},\gamma,\beta$ | 1252 | 84  | 4.2| 1253    | 39  | 5.5| 1261    | 30  | 6.1 |
| $\beta,\beta_{\text{OH}}$ | 1188 | 77  | 21 | 1183    | 31  | 3.6| 1173    | 278 | 2.5 |
| $\beta_{\text{OH}}$ | 1146    | 59 | 12 | 1147    | 100 | 8.5| 1156    | 57  | 3.3 |
| $\beta,\beta_{\text{OH}}$ | 1139 | 42  | 4.9| 1139    | 26  | 8.2| 1148    | 4.9  | 11 |
| $\gamma$          | 1092    | 53 | 2.6| 1090    | 65  | 10 | 1089    | 44  | 5.4 |
| $\gamma$          | 933     | 23 | 7.5| 938     | 34  | 5.8| 940     | 27  | 6.3 |
| $\rho$            | 931     | 6.7| 1.1| 910     | 0.9 | 1.0| 909     | 0.6 | 1.6 |
| $\rho$            | 824     | 32 | 7.1| 853     | 6.1 | 7.7| 822     | 22  | 4.6 |
| $\rho$            | 816     | 0.3| 1.1| 790     | 29  | 5.0| 793     | 18  | 3.9 |
| $\gamma$          | 785     | 11 | 11 | 782     | 7.1 | 3.6| 784     | 14  | 5.4 |
| $\gamma$          | 771     | 40 | 18 | 773     | 42  | 23 | 769     | 20  | 23 |
| $\gamma$          | 698     | 1.8| 0.9| 697     | 1.7 | 1.0| 698     | 1.3 | 0.8 |
| $\gamma$          | 621     | 9.6| 3.1| 627     | 6.1 | 3.2| 627     | 9.3 | 3.2 |
| $\gamma$          | 617     | 8.7| 1.3| 616     | 25  | 1.5| 616     | 15  | 1.5 |
| $\gamma$          | 582     | 13 | 3.9| 581     | 7.0 | 6.8| 575     | 8.0 | 4.4 |
| $\gamma$          | 456     | 4.5| 0.4| 456     | 0.1 | 0.3| 457     | 6.6 | 0.1 |
| $\gamma$          | 441     | 17 | 1.0| 441     | 5.8 | 0.9| 444     | 4.7 | 0.7 |
| $\gamma$          | 390     | 5.8| 1.4| 390     | 1.7 | 1.4| 352     | 101 | 5.8 |
| $\beta_{\text{CO}},\beta_{\text{OH}}$ | 309 | 14  | 1.2| 308     | 43  | 1.1| 310     | 23  | 1.7 |
| $\beta_{\text{CO}}$ | 295     | 19 | 1.4| 296     | 11  | 1.3| 307     | 35  | 3.1 |
| $\chi$            | 246     | 0.7| 2.6| 247     | 9.2 | 1.6| 279     | 12  | 0.4 |
### Vibrations of fragment \( \text{CHOH-CH}_2\text{NHCH}_3 \)

| \( \beta_{\text{CC}_{\text{OH}}} \) | 201 | 24 | 1.1 | 199 | 33 | 1.6 | 201 | 0.7 | 0.8 |
|----------------|-----|----|-----|-----|----|-----|-----|-----|-----|
| \( \chi \)    | 170 | 6.7 | 1.3 | 171 | 7.5 | 1.1 | 167 | 0.3 | 0.7 |

4. **Conclusions**

The carried modeling calculations of the vibrational state of rank 1,2,4 replaced benzol particulary dopamine and adrenaline allow us to confirm that the method of the density functional DFT/B3LYP can be used to construct structural and dynamical models of the complex molecule compounds of the given type. The given fundamental vibrations could be relatively divided into two groups. The first group is related to the vibrations of the benzol fragment \( \text{C}_6\text{H}_3\text{X}_3 \). If to carry out the mass compare (X=F, \( \text{CH}_3 \), OH) the vibrations could be considered as characteristic according to the frequency and form. Another group is related to the fundamental vibrations of a molecular fragment which is obtained by 4 varied molecular fragments .substitution of a hydrogen atom of a methyl group in a position.

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