Structurally-dynamic models of substituted benzoic acids

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Abstract. On the basis of modelling not empirical quantum calculations of geometrical and
electronic structure of some isomers of substituted benzoic acids are investigated regularity in
behaviour of parameters of the adiabatic potential a carboxyl fragment.

Keywords: benzoic acids, adiabatic potential, intermolecular interaction, oscillatory spectra.

1. Introduction
Substituted benzoic acids have wide enough application as reliable indicators of environmental
contamination by waste of mineral oil, components by manufacture of the pesticides making of
pharmacological preparations, dyes of textile manufactures. In detail about it, it is possible to learn from
the literary review in work [1].

Research of structure and spectra of the specified representatives aromatic benzoic acids one of stages
of studying of physical and chemical properties of the ligands (benzoic and salicylic acids) with metals
within the limits of new in the physic of molecules of a scientific direction - molecular modelling. A
theoretical basis of such researches are not empirical methods of quantum mechanics of molecular
systems.

Benzoic an acid, as well as other representatives of class carboxylic acids, easily form dimers with
strong hydrogen communications. Intermolecular interaction between monomers is evidently shown in
oscillatory spectra of connections. Especially it concerns a high-frequency range (2500-3500 см⁻¹). The
spectrum of dimers in this area has complex structure, including valent fluctuations of communications
СН benzoic a skeleton, OH bonds of carboxyl fragment and overtones of deformation fluctuations of the
specified communications. The theoretical interpretation of strips offered in the periodic literature, is
controversial, it is enough to refer to publications [2-6]. If to follow the presented results to them, property
of characteristical strips of carboxyl fragment, taking place for monomers of carboxylic acids, is
cardinally broken at formation dimers OH bonds.
For dimers of carboxylic acids and of some of its substituted interpretation of an oscillatory spectrum in overwhelming majority of researches is based on use of scaling parities [7], by updating results of modelling calculations in harmonious approach of the theory of molecular fluctuations [1].

As shown in the works [8-10], the results received on this way for a range of 2500-3500 sm\(^{-1}\) essentially miss the data received at the decision of a problem in inharmonious approach. Technique of the account offered in publications [9,10] inharmonic shift of the strips uses as initial data the decision of a problem on molecular fluctuations monomers of carboxylic acids. Interpretation of oscillatory spectra of monomers allows to identify the strips concerning valent fluctuations of communications CH of a base fragment (for example, the benzene skeleton) to estimate influence of intermolecular interaction on shift and splitting of strips at formation dimer bonds. The technique is approved on such representatives of a class carboxylic acids, as benzoic and isonicotinic acid [9-11].

Preliminary stage of construction of structurally-dynamic models substituted benzoic acids is the analysis of influence of electronic structure of the assistant on parameters of the adiabatic potential of carboxyl fragment depending on mutual position (ortho-, metha-, pair [12]) assistants concerning an aromatic ring. Such analysis also is a subject of the given publication.

2. Mathematical model of inharmonic shift of oscillatory conditions

For the description inharmonic shift of oscillatory conditions we shall take advantage of a parity for the description of molecular fluctuations within the limits of the theory of indignation [13].

\[
E^n = v_s \left( n_s + \frac{1}{2} \right) + \chi_{sr} \left( n_s + \frac{1}{2} \right) \left( n_r + \frac{1}{2} \right) .
\]

(1)

Corresponding modelling hamiltonian has, an appearance:

\[
H^{(v)} = \frac{1}{2} v_s (P_s^2 + (Q')^2) + \mu^{1/4} P_a \mu^{-1/4} P \mu^{1/4} + \frac{1}{3} F_{str} Q' Q' Q' + \frac{1}{12} F_{str} Q' Q' Q' Q'' .
\]

(2)

Here \( P_a = L(\alpha, sr) Q' P \); \( L(\alpha, sr) \) - Constants Coriolis, \( v_s \) - frequencies of harmonious fluctuations (in sm\(^{-1}\)); \( Q' \) - the dimensionless normal oscillatory coordinates linearly connected with the Cartesian displacement of atoms; \( F_{str} \) and \( F_{str} Q' \) - cubic and quartic force constants (parameters adiabatic potential of a molecule), \( n_s \) - quantum numbers of a considered oscillatory condition. The size of the inharmonic shift of a separate strip of fundamental fluctuation is defined by size inharmonic amendments \( X_{ss} = 2 \chi_{ss} \) and \( X_s = \chi_{sr} / 2 \). Expressions for inharmonic constants \( \chi_s \) are offered in publications [9,10].

\[
\chi_{ss} = \frac{1}{16} F_{sss} - \frac{5}{48} (F_{ss})^2 \left( \frac{1}{v_s} + \frac{1}{2} (F_{ss})^2 \left( \frac{1}{2 v_s - v_r} - \frac{1}{2 v_s + v_r} - \frac{4}{v_r} \right) \right)(1 - \delta_{sr} .
\]

(3)

\[
\chi_{sr} = \frac{1}{16} F_{ssr} - \frac{5}{8} (F_{ssr})^2 \left( \frac{1}{2 v_s - v_r} + \frac{1}{2 v_s + v_r} \right)(1 - \delta_{sr} +
\]

\[
+ \frac{3}{8} (F_{sr})^2 \left( \frac{1}{v_s + v_r + v_s} + \frac{1}{v_t - v_r - v_s} + \frac{1}{v_l - v_r + v_s} + \frac{1}{v_t + v_r - v_s} \right) \times
\]

\[
\times (1 - \delta_{sr})(1 - \delta_{sr})(1 - \delta_{sr} + \frac{1}{2} L(\alpha, sr) \frac{1}{v_s + v_r} \left( \frac{1}{v_s} + \frac{1}{v_r} \right)
\]

(4)
All set of fundamental fluctuations of substituted benzoic acid can be divided acids on two parts. The first part concerns to fluctuations of the benzene skeleton (C₆H₄). The received results concerning properties characteristical oscillation para-, meta- and ortho substituted benzenes will completely be coordinated with conclusions of the monography [12]. For chloro-and carboxy-benzoic acid such information is presented to publications [14] which basic purpose was research of influence of nuclear basis on results of modelling calculations of parameters adiabatic potential. It is found out, that the choice of basis influences predictive values of the frequencies calculated in harmonious approach valent and torsional vibrations of the OH carboxyl fragment. The preference should be given bases 6-311G **, 6-311+G **, 311+G ** [15]. Accounting for the diffusion parameters of the basis (+,++) shifts the frequency of torsional vibrations of OH in the low-frequency spectrum by ~ 30 cm⁻¹. Qualitative assessment of band intensities in IR and Raman preserved.

3. Results and discussion

The results of model calculations of the vibrational states of the carboxyl fragment of chlorine, cyano, hydroxy-and carboxy-benzoic acid (method of the functional density DFT/B3LYP with basis 6-311 + G **) are presented in Tables 1-6.

Characteristic frequency, form and intensity in the IR and Raman is the stretching vibrations of OH (QOH), for which there is practically no doublet splitting in dicarboxy benzenes. Characteristic frequency and intensity should recognize and respect, and oscillation of the C=O(QC=O).

For the other vibrations of the bands and their intensity depends, in varying degrees, the relative position of substitute and the carboxyl fragment.

In the para substituents of benzoic acid components of the influence of substitute impact on the strips interpreted as deformation fluctuation of valent corner COC (γOCO) of a carboxyl fragment (a range of values of 600-720 sm⁻¹). Significantly different estimates of the intensities of bands in the infrared spectrum. The remaining variations should be attributed to the characteristic frequency, if we neglect the divergence of the torsional vibrations of a doublet ρOH (Δ ~20 sm⁻¹). Such behavior of the fundamental frequency as compared with benzoic acid (X = H) is associated with spatial distance from the substitute-carboxyl frag (> 7 Å). The intensity of the stripes is defined by the electronic structure of substitute.

Intensity of strips is defined by an electronic structure of the substitute. Identification of isomers of hydroxy (OH) and carboxy (COOH) para substituents of benzoic acid is complicated (Table 1).

In metasubstituted benzoic acids are possible two isomers for substitutes X=Cl, CN (Table 2), four isomers, if X=OH (Table 3), three isomers for X=COOH (Table 4).

According to data of table 2, for such substitutes as Cl and CN spectral identification of the isomers in the para-and ortho-positions is difficult, which is also related to the long distance between the atoms of the X substituent and carboxyl fragment (> 5 Å for metasubstitution and 3.9 Å for parasubstitution).

Spectral identification of isomers of meta hydroxy substituted benzoic acid (Table 3) is complicated. Frequency shift, according to modelling calculations is 20 sm⁻¹, qualitative assessment of the intensity remains. The distance between the hydrogen atom of the hydroxyl moiety and the oxygen atoms of the carboxyl fragment exceeds the value of 4.7 Å.
Table 1. Interpretation of fluctuations of carboxyl a fragment vapor substituted benzoic acids (C₆H₄COOH)

| X= | The form | ν_{vib} | ν_e | ν_a | IR | Raman | The form | ν_{vib} | ν_e | ν_a | IR | Raman |
|----|----------|---------|-----|-----|----|-------|----------|---------|-----|-----|----|-------|
| H  |          | 3570    | 3772| 3577| 99 | 137   |          | 1325    | 1363| 1327| 116| 12 |
| Cl |          | 3581    | 3771| 3571| 111| 146   |          | 1358    | 1365| 1345| 136| 24 |
| CN |          | -       | 3769| 3580| 107| 174   |          | 1334    | 1378| 1336| 129| 20 |
| OH_1 | Q_OH | 3570    | 3774| 3584| 91 | 152   | β_OH    | 1325    | 1370| 1328| 127| 11 |
| OH_2 | Q_C-O | 3570    | 3774| 3584| 92 | 152   | Q_CO, β_OH | -      | 1380    | 1338| 147| 18 |
| COOH_1 |      | -       | 3768| 3579| 224| 322   | -        | -1365   | 1324| 243| 35 |
| COOH_2 |      | -       | 3770| 3580| 224| 323   | -        | -1364   | 1324| 240| 32 |
| H  |          | 1690    | 1785| 1753| 395| 92    |          | 1073    | 1114| 1088| 42 | 1.2 |
| Cl |          | 1698    | 1786| 1753| 418| 147   |          | 1095    | 1102| 1075| 222| 12 |
| CN |          | 1710    | 1808| 1747| 331| 93    |          | -       | 1110    | 1079| 133| 2.8 |
| OH_1 | Q_C-O | 1775    | 1797| 1737| 357| 88    | Q_CO, β_OH | -     | 1100    | 1070| 132| 1.1 |
| OH_2 |        | 1796    | 1735| 355  | 83 |       |          | -       | 1106    | 1075| 192| 2.1 |
| COOH_1 |      | 1789    | 1727| 800  | 260| 60    | -        | -1104   | 1073| 359| 12 |
| COOH_2 |      | 1790    | 1730| 774  | 264| 60    | -        | -1103   | 1072| 336| 7.2 |
| H  |          | 640     | 634 | 49   | 0.4| 571   |          | 578     | 577| 71  | 2.5 |
| Cl |          | 677     | 668 | 14   | 0.7| 549   |          | 577     | 571| 59  | 3.1 |
| CN |          | 691     | 705 | 687  | 41 | 1.3   |          | 588     | 605| 591| 28 | 3.2 |
| OH_1 | γ_C-O | 630     | 603 | 589  | 58 | 0.5   |          | 560     | 591| 577| 49 | 6.9 |
| OH_2 | γ_C-O | -       | 602 | 588  | 62 | 0.4   | ρ_OH    | -       | 572     | 578| 48  | 7.1 |
|      |        | -       | 720 | 701  | 102| 0     |          | -       | 591     | 577| 134| 00 |
| COOH_1 |      | -       | 646 | 630  | 0  | 7.5   | -        | -670    | 557| 0   | 5.5 |
| COOH_2 |      | -       | 719 | 701  | 92 | 1.6   | -        | -589    | 575| 134| 0.2 |
|      |        | -       | 646 | 630  | 0.7| 8.6   | -        | -570    | 557| 0   | 5.4 |

The note. Frequencies of fluctuations in sm⁻¹, intensity in spectra IR in KmA/m, in Raman spectra in Å²/amu.
Table 2. Interpretation of fluctuations carboxil fragment the metha-and ortho- substituted benzoic acids (C₆H₄COOH_X. X=Cl, CN)

| Form       | X=    | νᵣ | νₓₓₓ | Isomer_1 | Isomer_2 | νᵣ | νₓₓₓ | Isomer_1 | Isomer_2 |
|------------|-------|----|-----|----------|----------|----|-----|----------|----------|
|            |       | IR | Raman |          |          | IR | Raman |          |          |
| QOH        | Cl    | 3742 | 3556 | 64       | 166      | 65 | 175 | 3725     | 3539     | 55       | 164     | 65       | 152     |
|            | CN    | 3770 | 3581 | 103      | 157      | 104 | 167 | 3766     | 3577     | 104      | 144     | 104      | 147     |
| QCO        | Cl    | 1808 | 1747 | 333      | 57       | 310 | 55  | 1788     | 1728     | 344      | 41      | 298      | 52      |
|            | CN    | 1810 | 1749 | 333      | 54       | 296 | 54  | 1799     | 1768     | 316      | 51      | 254      | 45      |
| βOH        | Cl    | 1383 | 1341 | 105      | 8.8      | 89  | 7.6 | 1396     | 1353     | 87       | 10      | 57       | 6.5     |
|            | CN    | 1381 | 1338 | 128      | 16       | 95  | 14  | 1381     | 1340     | 124      | 13      | 95       | 9.9     |
| QCO        | Cl    | 1096 | 1066 | 98       | 1.7      | 19  | 7.2 | 1126     | 1095     | 96       | 0.5     | 68       | 2.9     |
|            | CN    | 1098 | 1088 | 99       | 1.2      | 52  | 2.8 | 1137     | 1105     | 119      | 1.3     | 85       | 0.9     |
| γOCO       | Cl    | 647  | 631  | 41       | 0.1      | 46  | 2.4 | 642      | 627      | 41       | 3.4     | 45       | 0.2     |
|            | CN    | 652  | 636  | 42       | 0.2      | 52  | 2.4 | 642      | 627      | 39       | 2.7     | 40       | 0.2     |
| ρOH        | Cl    | 627  | 612  | 104      | 6.1      | 108 | 5.5 | 631      | 616      | 57       | 6.7     | 76       | 7.4     |
|            | CN    | 623  | 608  | 91       | 6.4      | 89  | 7.8 | 595      | 581      | 72       | 5.1     | 57       | 4.2     |

Table 3. Interpretation of oscillations of carboxi fragment meta hydroxy substituted benzoic acids

| Form       | Isomer_1 | Isomer_2 | Isomer_3 | Isomer_4 |
|------------|----------|----------|----------|----------|
|            | νₓₓₓ IR Raman | νₓₓₓ IR Raman | νₓₓₓ IR Raman | νₓₓₓ IR Raman |
| QOH        | 3638 63 123 | 3636 59 101 | 3635 61 99  | 3637 63 122 |
| QOH        | 3583 88 154 | 3582 88 151 | 3581 90 153 | 3581 88 155 |
| QCO        | 1742 308 57 | 1743 318 59 | 1738 316 59 | 1743 314 56 |
| βOH        | 1337 131 16 | 1336 123 19 | 1340 109 14 | 1335 172 13 |
| QCO,βOH    | 1321 21 0.6 | 1324 28 2.1 | 1325 38 1.8 | 1321 14 0.5 |
| ρOH        | 1251 51 17 | 1253 69 17  | 1249 83 14  | 1250 36 15  |
| QCO,β      | 1058 87 1.1 | 1054 84 1.2 | 1084 99 0.7 | 1075 44 0.9 |
| βCO₂,γ     | 633 44 0.1 | 634 42 0.2 | 629 45 2.6 | 628 48 2.2 |
| χOH        | 597 96 5.4 | 596 89 5.5 | 601 87 5.2 | 601 96 5.2 |
| χOH        | 326 108 3.1 | 349 109 2.5 | 356 112 2.5 | 326 107 3.1 |
For isomers of metacarboxybenzen holds the doublet splitting of the band, interpreted as a deformation vibration of the bond angle $\beta_{COH}$ carboxyl fragment ($\sim 20$ cm$^{-1}$).

Significantly different intensities of the bands in the infrared spectrum for the isomers. Possible to identify the isomer of the intensity of the band, interpreted as stretching vibrations of C = O.

Table 4. Interpreting oscillations of the carboxyl fragment of metadicarboxibenzene

| Form         | Symbol type | Isomer 1 | | Isomer 2 | | Isomer 3 | | v$_{\text{sym}}$ | IR | Raman | v$_{\text{sym}}$ | IR | Raman | v$_{\text{sym}}$ | IR | Raman |
|--------------|-------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| q$_{OH}$     | A'          | 3580     | 88       | 171      | A1       | 3581     | 22       | 282      | 3582     | 83       | 190      |
| q$_{OH}$     | A'          | 3580     | 128      | 127      | B2       | 3581     | 193      | 22       | 3582     | 132      | 99       |
| Q$_{CO}$     | A'          | 1730     | 343      | 98       | A1       | 1739     | 697      | 124      | 1732     | 119      | 174      |
| Q$_{CO}$     | A'          | 1727     | 434      | 83       | B2       | 1728     | 16       | 49       | 1725     | 712      | 12       |
| $\beta_{COH}$, Q$_{CO}$ | A'          | 1334     | 67       | 24       | A1       | 1327     | 3.4      | 24       | 1339     | 199      | 24       |
| $\beta_{COH}$, Q$_{CO}$ | A'          | 1315     | 78       | 5.1      | B2       | 1318     | 86       | 1.5      | 1317     | 61       | 0.1      |
| Q$_{CO}$, $\beta_{COH}$ | A'          | 1092     | 112      | 0.4      | A1       | 1089     | 0.1      | 1.6      | 1107     | 125      | 0.5      |
| Q$_{CO}$, $\beta_{COH}$ | A'          | 1063     | 131      | 1.2      | A1       | 1077     | 46       | 1.5      | 1059     | 232      | 1.1      |
| $\gamma_{OCO}$ | A'          | 629      | 51       | 0.6      | A1       | 626      | 1.5      | 4.6      | 630      | 42       | 1.1      |
| $\gamma_{OCO}$ | A'          | 626      | 71       | 2.7      | B2       | 627      | 132      | 0.6      | 629      | 57       | 0.1      |
| $\rho_{OH}$  | A"         | 577      | 0.7      | 3.3      | A2       | 579      | 0       | 4.1      | 576      | 0        | 2.6      |
| $\rho_{OH}$  | A"         | 555      | 164      | 1.1      | B1       | 552      | 170      | 0.5      | 555      | 160      | 1.8      |

Orthohidroxisbiisstuted isomers of benzoic acid can be identified as on the bands ($\Delta \sim 50$ cm$^{-1}$), interpreted as a deformation vibration of the valence angle $\beta_{COH}$ and stretching vibrations of the CO carboxyl fragment, and on the intensities in the IR and Raman. Izomers_2 and 3 can be easily identified by their band, interpreted as stretching vibrations of OH hydroxyl fragment (q$_{OH}$).

The shift of this stripe to the low-frequency region by $\sim 120$ cm$^{-1}$ for izomer_2 and $\sim 300$ cm$^{-1}$ for izomer_3 associated with the presence of an intramolecular interaction between the oxygen atom of C = O and CO, respectively, the carboxyl group and a hydrogen atom of the hydroxyl fragment (R$_{OH}$ $\sim 1.75$ Å).

There is reason to believe that the mechanism of this interaction is the intramolecular hydrogen bond.

Results of the simulation of the adiabatic potentials of orthodicarboxibenzo are represented interesting (Table 6).

Torsional low-frequency vibrations of carboxyl fragments are reproduced only for the original non-planar configuration of the compound (the angle between the carboxyl fragments of $\sim 53^\circ$, the angle between the carboxyl fragment and the plane of the benzene ring $\sim 38^\circ$). Geometry optimization indicates the presence of one isomer of C2 symmetry. Doublet splitting is only important for the band, interpreted as the stretching vibration of CO bond. For the range below 1700 cm$^{-1}$ in the IR spectrum the most intense antisymmetric vibrations in the Raman spectrum – symmetric.
Table 5. Interpretation of fluctuations of the carboxyl fragment ortho-hydroxi-substituted benzoic acids

| Form | Isomer 1 | Isomer 2 | Isomer 3 | Isomer 4 |
|------|----------|----------|----------|----------|
|      | $\nu_{\text{IR}}$ | $\nu_{\text{Raman}}$ | $\nu_{\text{IR}}$ | $\nu_{\text{Raman}}$ | $\nu_{\text{IR}}$ | $\nu_{\text{Raman}}$ | $\nu_{\text{IR}}$ | $\nu_{\text{Raman}}$ |
| $q_{\text{OHg}}$ | 3627 | 61 | 114 | 3507 | 286 | 91 | 3188 | 306 | 65 | 3623 | 58 | 123 |
| Q_{\text{OH}} | 3569 | 76 | 158 | 3581 | 76 | 142 | 3570 | 106 | 144 | 3588 | 85 | 148 |
| Q_{\text{C-O}} | 1721 | 356 | 44 | 1750 | 391 | 61 | 1683 | 392 | 57 | 1749 | 362 | 61 |
| $\beta_{\text{COH}}$ | 1341 | 85 | 7.5 | 1371 | 44 | 5.4 | 1393 | 169 | 16 | 1331 | 89 | 4.1 |
| $\beta, \beta_{\text{COH}}$ | 1324 | 49 | 2.1 | 1315 | 41 | 8.9 | 1358 | 76 | 6.7 | 1319 | 35 | 4.9 |
| $q_{\text{CO}, Q}$ | 1246 | 47 | 9.9 | 1240 | 125 | 3.2 | 1267 | 61 | 2.1 | 1260 | 22 | 6.6 |
| Q_{\text{CO}} | 1102 | 182 | 1.4 | 1054 | 97 | 8.6 | 1064 | 59 | 1.3 | 1114 | 97 | 0.1 |
| $\beta_{\text{OCO}}, \gamma$ | 627 | 45 | 2.7 | 622 | 41 | 2.3 | 639 | 52 | 0.4 | 631 | 44 | 0.1 |
| $\chi_{\text{CO}, \chi}$ | 586 | 64 | 5.5 | 547 | 152 | 5.7 | 573 | 81 | 6.4 | 572 | 82 | 7.0 |

Table 6. Interpretation of oscillatory conditions orthodicarboxsibenzol

| Form | $\nu_{\text{scen}}$ [16] | $\nu_{\text{v}}$ | $\nu_{\text{IR}}$ | $\nu_{\text{Raman}}$ | $\nu_{\text{scen}}$ [16] | $\nu_{\text{v}}$ | $\nu_{\text{IR}}$ | $\nu_{\text{Raman}}$ |
|------|-----------------|----------------|----------------|----------------|-----------------|----------------|----------------|----------------|
|      | Symmetry type A | Symmetry type B |
| $q_{\text{OH}}$ | 3570 | 3761 | 3573 | 98 | 198 | - | 3761 | 3572 | 88 | 110 |
| Q_{\text{C-O}} | 1760 | 1814 | 1753 | 358 | 68 | - | 1794 | 1734 | 310 | 28 |
| $\beta_{\text{COH}}$ | 1325 | 1363 | 1322 | 69 | 11 | 1306 | 1359 | 1318 | 126 | 3.1 |
| Q_{\text{CO}}, $\beta_{\text{COH}}$ | 1070 | 1114 | 1082 | 23 | 2.8 | 1051 | 1065 | 1036 | 202 | 0.4 |
| $\gamma_{\text{OCO}}$ | 630 | 641 | 625 | 25 | 2.9 | - | 639 | 624 | 65 | 0.5 |
| $\rho_{\text{OH}}$ | 570 | 598 | 584 | 24 | 2.1 | - | 602 | 588 | 116 | 2.3 |

4. Conclusion

Comparison of the results of model calculations of the geometric structure and vibrational states of substituted benzoic acid monomer with various electron-donating properties with available experimental data gives basis to assert that the density functional method DFT/B3LYP allows carries out accurate predictive calculations of geometric and electronic structure of the investigated class of compounds and use them to build a structurally dynamic models.

References

[1] Mukherjeea V, Singha N P, Yadavb R A 2010 FTIR and Raman spectra and optimized geometry of 2,3,6-tri-fluorobenzoic acid dimer: A DFT and SQMFF study *Spectrochim. Acta* 77A (4) 787-794.
[2] Florio G M, Zwier T S, Myshakin E M, Jordan K D, Sibert E L 2003 Theoretical modeling of the OH stretch infrared spectrum of carboxylic acid dimmers on first-principles anharmonic coupling J.Chem. Physic. 118(4) 1735-1746

[3] Antony J, Helden G, Meijer G, Schmidt B 2005 Anharmonic midinfrared vibrational spectra of benzoic acid monomer and dimmer J.ChemPhysics 123 014305 pp 1-11

[4] Matanovic L, Doslic N 2007 Theoretical modeling of formic acid dimer infrared spectrum. Shaping the O-H stretch bond Chemical Physics. 338 121-126.

[5] Olbert-Majrat A, Ahokas J, Lundell J, Pettersson M 2009 Raman spectroscopy of formic acid and its dimmers isolated in low temperature argon matrices Chemical Physics Letters 468 176-183.

[6] Durlak P, Latajka Z 2009 Cal-Parinello molecular dynamics and density functional Theory simulation of infrared spectra for acetic acid monomers and cyclic dimers Chemical Physics Letters 477 249-264.

[7] Krasnoshchekov S V, Stepanov N F 2007 Scale factors as effective parameters for correcting nonempirical force fields Russian Journal of Physical Chemistry A 81 (4) 680-689.

[8] Elkin M D, Shalnova T A, Pulin V F 2009 Adiabatic potential modelling of carboxylic acids Bulletin Saratov State University 1 (37) 109-114.

[9] Elkin M D, Nuraliev D M, Djalmuhambetova E A, Gaysina A R, Alykova O M 2012 Systematic analysis of model calculations for the adiabatic potential of the dimers of carboxylic acids. Caspian Journal: Management and high technologies. 1(17) 118-125.

[10] Elkin M D, Pulin V F, Osin A B 2010 Mathematical's Aspens of model in molecular modelling Bulletin Saratov State University. 4(49) 36-39.

[11] Sanchez E, Nariez J L, Martinez F 1986 Vibrational spectra of some o-substituted benzoic acid derivatives J. Mol. Struct. 142 45-48.

[12] Sverdlov L M, Kovner M A, Krajnov E P 1970 Vibrational spectra of multiatomic molecules (Moscow: A science) p. 550.

[13] Hoy A R, Mills I M, Strey G 1972 Anharmonic force constants calculation J. Mol. Phys. 21(6) 1265-1290.

[14] Erman E A, Elkin M D, Grechukhina O N, Lihkter A M 2011 Modeling the structure and spectra of substituted benzoic acid Natural sciences. 1(34) 206-212.

[15] Frisch M J, Trucks G W, Schlegel H B et al 2003 Gaussian 03. Revision B.03. (Pittsburg PA.: Gaussian Inc.)

[16] Sanchez E, Nariez J L, Martinez F 1986 Vibrational spectra of some o-substituted benzoic acid derivatives J. Mol. Struct. 142 45-48.