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# Investigation of the dynamics of the 3-methylpyridine molecule based on Raman scattering, infrared absorption spectra, and theoretical calculations

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**Abstract.** The structure and vibrational dynamics of the 3-methylpyridine ($C_5H_4N(CH_3)$) molecule were investigated using Raman scattering and infrared absorption spectra, as well as theoretical calculation results based on the (DFT) method and the (B3LYP) HF/6-311G$^{**}$ basis set. The contribution of the $CH_3$ group to the Raman spectrum was studied by comparing the 3-methylpyridine molecule with pyridine. The shift of the spectral line associated with the vibration of the pyridine ring towards higher frequencies in the low-frequency range (100-1043 cm$^{-1}$) and the shift of the spectral lines resulting from the rotational-twisting movements of the pyridine ring towards lower frequencies were discussed.

## INTRODUCTION

Obtaining accurate information about intermolecular interaction forces and their nature in condensed media, investigating the mechanisms of manifestation of optical spectra in molecules with complex atomic arrangements, and drawing scientifically grounded conclusions about molecular structures are among the fundamental and practical directions of spectroscopic research. Our research work is a logical continuation of studies in this direction, dedicated to investigating the relaxation regularities at energy levels.

Below, we will focus on the analysis of certain experimental and theoretical works relevant to our research.

Despite the extensive study of the structures of pyridine and its derivatives, which are considered organic heterocyclic compounds, the number of spectroscopic studies dedicated to them continues to grow annually due to their wide application in pharmacology, agrochemistry, and many other fields. The Raman scattering (RS) and infrared (IR) absorption spectra of various pyridine derivatives have been studied through both experimental and quantum-chemical theoretical calculations, analyzing the different characteristics of the spectra [1-6]. The spectral properties of pyridine for atmospheric monitoring have been identified using IR absorption spectra for the gas phase of pyridine [7]. The frequency shift of the Rayleigh scattering spectrums Mandelstam-Brillouin component in aqueous solutions of γ-picoline has been studied in relation to temperature and concentration [8]. The bond length and valence vibration frequency of the B-N bond in the pyridine-borane molecule, as well as the effect of complex formation on pyridine, have been demonstrated [9]. Molecular clustering regularities in pyridine, aniline, and their solutions have been studied using the RS spectra [10,11]. The frequency shifts and line width changes of the spectral lines in the 960-1080 cm$^{-1}$ and 2700-3650 cm$^{-1}$ ranges in mixtures of pyridine with methanol at various relative concentrations have been discussed in relation to pyridine concentration [12].

Raman spectra resulting from vibrational and rotational movements of molecules in aromatic hydrocarbons with symmetric and asymmetric polarizability tensors have been studied, providing detailed information on the mechanisms of optical spectrum manifestation based on the analysis of the obtained results. The frequencies of the RS spectra have been theoretically calculated and compared with experimental results based on these findings [13,14,15].

The Raman spectra of multi-atomic organic molecules such as acetone, neopentane, and ethylene explain several characteristic features of the vibrations of $CH_3$ and $CH_2$ groups [16].

For simple alcohols (from n-pentanol to n-decanol), it has been determined that the spectral lines in the Raman spectra in the low-frequency range of 200-600 $cm^{-1}$ are related to the twisting and bending vibrations of the groups formed by the increasing number of carbon atoms in the hydrocarbon chain [17]. The Raman spectrum of n-butane has spectral lines at 116.60 $cm^{-1}$ and 121.28 $cm^{-1}$ in the low-frequency range, which are associated with asymmetric twisting vibrations [18]. The following authors [19] have evaluated the short frequency range of 1550-1900 $cm^{-1}$ in Raman spectra as a “fingerprint within a fingerprint” region for identifying pharmaceutical ingredients in drugs.

Despite the abundance of experimental and theoretical data on the regularities of various physical properties of pyridines with a methyl group in the molecular structure, there is currently no unified view on the molecular-level processes occurring in these liquids and their manifestation in RS spectra. This indicates the need for further extensive research on these objects.

Based on the above considerations, this study investigates the structure and vibrational regularities of the 3-methylpyridine ($C_5H_4N(CH_3)$) molecule by comparing its RS and IR absorption spectra, as well as theoretical quantum-chemical calculation results, with those of pyridine ($C_5H_5N$). The contribution of the $CH_3$ group to the Raman spectrum of the 3-methylpyridine molecule is examined.

## EXPERIMENTAL RESEARCH

3-methylpyridine was purchased by the “Sigma-Aldrich” company in the USA. Its purity is 99.5%, and it was used for recording spectra without additional purification. The RS spectra of the research objects were recorded on a spectrometer created on the basis of the InVia Raman spectrometer from “Renishaw” company (in the frequency range of 100 – 4000 $cm^{-1}$). The spectral resolution of the Raman spectrometer is 0.3 $cm^{-1}$, and the spatial resolution is 0.25 μm. Lasers with a power of 100 mW and wavelengths of 532 nm and 785 nm were used as light sources. The IR absorption spectra were recorded on the Spectrum Two IQ-Fure spectrometer (in the range of 400 – 4000 $cm^{-1}$).

The optimal geometric parameters and theoretically calculated Raman spectrum of the 3-methylpyridine molecule were obtained using the ORCA software, based on the density functional theory (DFT) method and the (B3LYP) HF/6-311G$^{**}$ basis set [20].

## RESEARCH RESULTS

**Experimental RS spectra selected for analysis.** The RS spectra for the research objects were recorded using laser radiation in the visible (λ=532 nm) and near-infrared (λ=785 nm) regions, with the frequency distribution of the spectra shown in Figures 1 and 2.

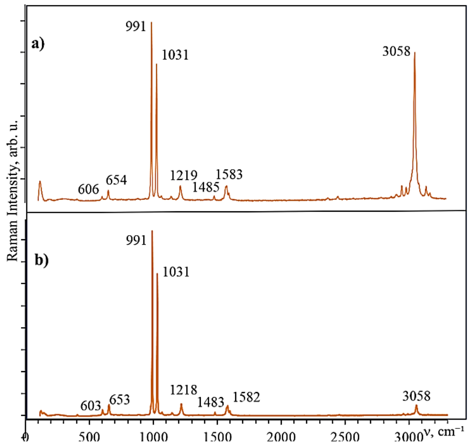

**FIGURE 1.** RS spectra for pyridine: a) laser-532 nm, laser power-10%; b) laser-785 nm, laser power 10%.

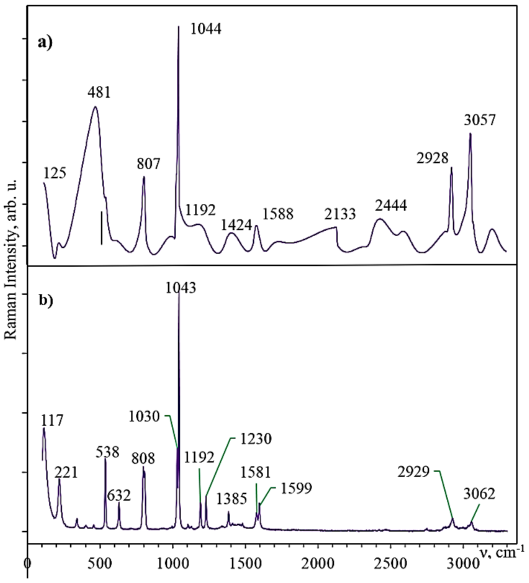

**FIGURE** 2. RS spectra for 3-methylpyridine: a) laser-532 nm, laser power-10%; b) laser-785 nm, laser power 10%.

According to the analysis of Figures 1 and 2, the fluorescence effects influence on the RS spectrum was observed in 3-methylpyridine, whereas no fluorescence was observed in pyridine. Therefore, in the analysis of the RS spectra, the spectrum obtained using laser radiation with a wavelength of 532 nm was used for pyridine, and the spectrum obtained using laser radiation with a wavelength of 785 nm was used for 3-methylpyridine.

**Results of the calculation of the optimal geometric parameters of the 3-methylpyridine molecule.** The 3-methylpyridine molecule is a derivative formed by the substitution of a methyl group ($CH_3$) for one hydrogen in the pyridine ring. Fig.3 shows the structural model of the 3-methylpyridine molecule. The optimized geometric parameters of the 3-methylpyridine molecule are given in Table 1.

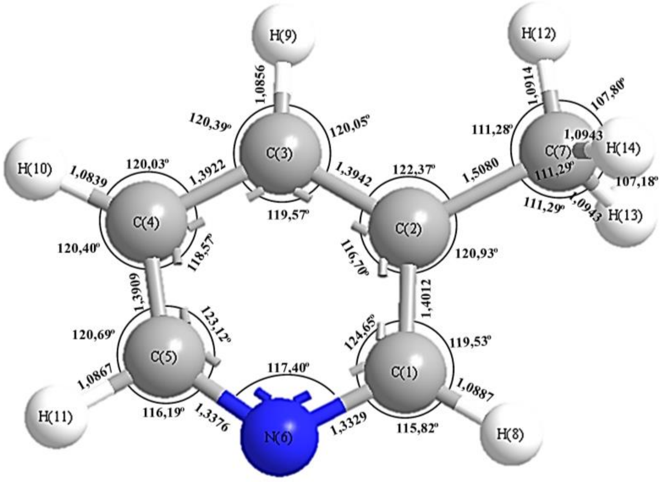

**FIGURE 3**. 3-Methylpyridine molecular structure model.

**TABLE1.** Theoretically calculated optimal geometric parameters of the 3-methylpyridine molecule

| Bond between atoms | Bond length (Å) | Bond between atoms | Bond angle ($^0$) | Bond between atoms | Dihedral angle ($^0$) |
|---|---|---|---|---|---|
| C1–C2 | 1.4012 | N6-C1-H8 | 115.82 | C3-C2-C1-H8 | -180 |
| C2–C3 | 1.3942 | C2-C1-N6 | 124.65 | C3-C2-C1-N6 | 0 |
| C3–C4 | 1.3922 | C2-C1-H8 | 119.53 | C7-C2-C1-H8 | 0 |
| C4–C5 | 1.3909 | C1-C2-C3 | 116.70 | C7-C2-C1-N6 | -180 |
| C5–N6 | 1.3376 | C3-C2-C7 | 122.37 | H9-C3-C2-C1 | 180 |
| N6–C1 | 1.3329 | C1-C2-C7 | 120.93 | C4-C3-C2-C7 | 180 |
| C2–C7 | 1.5080 | C4-C3-H9 | 120.39 | C4-C3-C2-C1 | -0 |
| H8–C1 | 1.0887 | C2-C3-C4 | 119.57 | C4-C3-C2-C7 | -0 |
| H9–C3 | 1.0856 | C2-C3-H9 | 120.05 | H10-C4-C3-H9 | 0 |
| H10–C4 | 1.0839 | C5-C4-H10 | 120.40 | H10-C4-C3-C2 | 180 |
| H11–C5 | 1.0867 | C3-C4-H10 | 121.03 | C5-C4-C3-H9 | -180 |
| H12–C7 | 1.0914 | C3-C4-C5 | 118.57 | C5-C4-C3-C2 | 0 |
| H13–C7 | 1.0943 | C4-C5-H11 | 120.69 | H11-C5-C4-C3 | 180 |
| H14–C7 | 1.0943 | C4-C5-N6 | 123.12 | N6-C5-C4-H10 | -180 |
|  |  | N6-C5-H11 | 116.19 | N6-C5-C4-C3 | 0 |
|  |  | C1-N6-C5 | 117.40 | H11-C5-C4-H10 | 0 |
|  |  | H13-C7-H14 | 107.18 | C1-N6-C5-H11 | -180 |
|  |  | H12-C7-H14 | 107.80 | C1-N6-C5-C4 | -0 |
|  |  | C2-C7-H14 | 111.29 | C5-N6-C1-H8 | 180 |
|  |  | H12-C7-H13 | 107.80 | C5-N6-C1-C2 | -0 |
|  |  | C2-C7-H13 | 111.29 | H14-C7-C2-C3 | 120.27 |
|  |  | H12-C7-H12 | 111.28 | H14-C7-C2-C1 | -59.73 |
|  |  |  |  | H13-C7-C2-C3 | -120.24 |
|  |  |  |  | H13-C7-C2-C1 | 59.76 |
|  |  |  |  | H12-C7-C2-C3 | 0.01 |
|  |  |  |  | H12-C7-C2-C1 | -179.99 |

From the analysis of Table 1, it is evident that among the C–C bonds in the 3-methylpyridine molecule, the C2 - C3 and C1 - C2 bond lengths are the longest, extending by 0.0030 Å and 0.007 Å respectively compared to the bond lengths in the pyridine molecule [15]. The shortest bond is the C4 - C5 bond, which is shortened by 0.002 Å. The H9 – C3 and H8 - C1 bonds are extended by 0.001 Å. The N6 - C1 bond length is extended by 0.003 Å, while the C5 - N6 bond length is shortened by 0.004 Å. The angle of the methyl group introduced into the pyridine ring decreased by 2°, while the adjacent C2-C1-N6 and C2-C3-C4 angles increased by 1°. Among the bond distances, the distance between the C2 –C7 atoms is the largest, measured at 1.5080 Å. These changes in the pyridine ring are related to the introduction of the electron-donor $CH_3$ group.

**Results of RS analysis, IR absorption and theoretical calculated spectra obtained for the 3-methylpyridine molecule.** Fig.4 illustrates the general view of the experimental RS and IR absorption spectra in the wavenumber range of 0-3500 $cm^{-1}$ for the 3-methylpyridine molecule. An overview of the theoretically calculated and experimentally obtained Raman spectra of the 3-methylpyridine molecule is presented in Fig.5. The experimental results are included in Table 2.

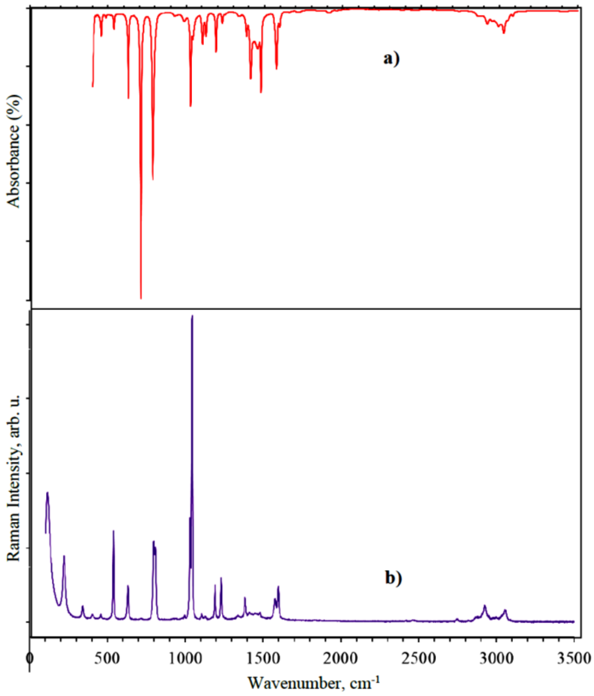

**FIGURE 4.** for 3-methylpyridine obtained experimentally: a) IR absorption spectrum, b) RS spectrum

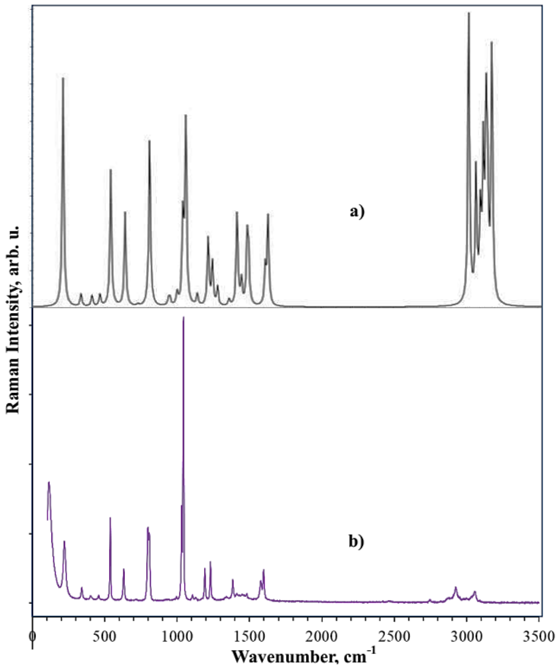

**FIGURE 5.** For 3-methylpyridine: a) Theoretically calculated RS spectrum, b) Experimentally obtained RS spectrum

**TABLE 2.** Experimental and theoretically calculated normal vibrational wavenumbers of the 3-methylpyridine molecule.

| № | Experimentally obtained wave number value, cm$^{-1}$ | | Theoretically calculated wave number value ν, cm$^{-1}$ | | |
|---|---|---|---|---|---|
| | RS | IR | ν | RS a. | IR a. |
| 1 | 117 | - | - | 0 | 0 |
| 2 | 221 | - | 212 | 2.533 | 1.520 |
| 3 | 341 | - | 335 | 0.282 | 0.260 |
| 4 | 415 | 401 | 410 | 0.333 | 3.706 |
| 5 | 464 | 456 | 468 | 0.433 | 0.306 |
| 6 | 538 | 538 | 544 | 6.199 | 5.072 |
| 7 | 632 | 630 | 643 | 5.336 | 32,916 |
| 8 | - | 710 | 731 | 0.117 | 20,472 |
| 9 | - | 787 | 799 | 0.311 | 1.150 |
| 10 | 808 | - | 812 | 12,887 | 0.586 |
| 11 | - | - | 944 | 0.603 | 0.005 |
| 12 | - | - | 951 | 0.724 | 0.208 |
| 13 | - | - | 998 | 0.131 | 5.590 |
| 14 | - | - | 1001 | 1.166 | 11,562 |
| 15 | 1030 | 1029 | 1041 | 9.385 | 11,562 |
| 16 | 1043 | 1042 | 1064 | 20.491 | 0.304 |
| 17 | 1107 | 1107 | 1065 | 0.035 | 4.376 |
| 18 | 1127 | 1128 | 1142 | 1.440 | 8.0003 |
| 19 | 1192 | 1192 | 1216 | 9.134 | 4.905 |
| 20 | 1230 | 1230 | 1245 | 6.106 | 2.979 |
| 21 | - | - | 1283 | 2.712 | 1.045 |
| 22 | - | - | 1363 | 1.033 | 1.478 |
| 23 | 1385 | 1384 | 1416 | 15,690 | 0.547 |
| 24 | - | 1413 | 1445 | 4.315 | 11.013 |
| 25 | - | 1456 | 1487 | 12.041 | 9.404 |
| 26 | - | 1479 | 1497 | 7,973 | 18.336 |
| 27 | 1581 | 1578 | 1510 | 0.310 | 12,726 |
| 28 | 1596 | 1596 | 1613 | 7,958 | 16,791 |
| 29 | - | - | 1633 | 18,840 | 0.573 |
| 30 | 2929 | 2927 | 3023 | 194.316 | 22,592 |
| 31 | 3062 | 3028 | 3074 | 90.233 | 15.204 |
| 32 | - | - | 3101 | 59,796 | 14,969 |
| 33 | - | - | 3120 | 104.931 | 33,909 |
| 34 | - | - | 3141 | 127,942 | 9.6010 |
| 35 | - | - | 3154 | 70,570 | 17.362 |
| 36 | - | - | 3182 | 189.903 | 17.232 |

According to the research results, 13 spectral lines with varying intensities were observed in the RS spectrum of the 3-methylpyridine molecule in the frequency range of 100–3500 cm$^{-1}$. The analysis of these spectral lines is provided below.

For heterocyclic aromatic compounds, the spectral lines related to the valence vibrations of the C-H bond are found in the 3000–3100 cm$^{-1}$ frequency range in the RS spectrum [21, 22, 23]. The spectral line at 3062 cm$^{-1}$ in the RS spectrum corresponds to the valence vibrations of the C-H bonds in the pyridine ring, appearing at 3028 cm$^{-1}$ in the IR absorption spectrum and at 3074 cm$^{-1}$ in the theoretical calculations. Literature [21, 22] indicates that the spectral line associated with the valence vibrations of the $CH_3$ group is at a lower frequency range of 2870–2962 cm$^{-1}$ compared to the valence vibrations of the CH bonds in the pyridine ring. In the RS spectrum, the spectral line related to the symmetric valence vibrations of the methyl group is observed at 2929 cm$^{-1}$, at 2927 cm$^{-1}$ in the IR spectrum, and at 3023 cm$^{-1}$ in the theoretical spectrum.

The valence vibrations related to the CC bond of the pyridine ring should be observed in the frequency range of 1750–1450 cm$^{-1}$ [22, 23]. In our study, spectral lines related to these vibrations were observed at 1581 cm$^{-1}$ and 1596 cm$^{-1}$ in the RS spectrum, at 1479 cm$^{-1}$, 1578 cm$^{-1}$, and 1596 cm$^{-1}$ in the IR spectrum, and at 1487 cm$^{-1}$, 1497 cm$^{-1}$, and 1613 cm$^{-1}$ in the theoretical calculations.

The spectral line observed at 1385 cm$^{-1}$ in the RS spectrum is related to the symmetric deformation vibrations of the CH$_3$ group, corresponding to 1384 cm$^{-1}$ in the IR spectrum and 1416 cm$^{-1}$ in the theoretical spectrum, confirming that these lines are related to symmetric deformation vibrations.

In the frequency range of 1000–1250 cm$^{-1}$, the in-plane deformation vibrations of the aromatic ring CH bond are exhibited [22]. The spectral lines at 1192 cm$^{-1}$ and 1230 cm$^{-1}$ in the experimentally obtained RS spectrum, at 1192 cm$^{-1}$ and 1230 cm$^{-1}$ in the IR absorption spectrum, and at 1216 cm$^{-1}$ and 1245 cm$^{-1}$ in the theoretical calculations were considered to be related to the in-plane deformation vibrations of the CH bond.

The spectral lines at 1030 cm$^{-1}$ and 1043 cm$^{-1}$ in the experimental data correspond to the asymmetric and symmetric (ring breathing) stretching vibrations of the pyridine ring, respectively. The spectral line at 1043 cm$^{-1}$ in the Raman scattering (RS) of 3-methylpyridine corresponds to the spectral line at 992 cm$^{-1}$ in the Raman scattering (RS) of pyridine, showing a shift of +51 cm$^{-1}$ to higher frequencies. This blue shift in the spectral line may be due to intermolecular interactions between the N atom of the 3-methylpyridine molecule and the H atoms of the neighboring molecule's methyl group. These spectral lines correspond to frequencies of 1029 cm$^{-1}$ and 1041 cm$^{-1}$ in the IR absorption spectrum, and to frequencies of 1042 cm$^{-1}$ and 1064 cm$^{-1}$ in the theoretical calculations.

The spectral line at 808 cm$^{-1}$ is associated with out-of-plane deformation vibrations of the H atoms in the methyl group. In the theoretical calculations, this line appears at 812 cm$^{-1}$, showing good agreement between the experimental and theoretical results.

The spectral lines at 538 cm$^{-1}$ and 632 cm$^{-1}$, which fall within the lower frequency range, are related to the rotational-twisting movements of the pyridine ring in the studied molecule. These lines have shifted to lower frequencies by -68 cm$^{-1}$ and -22 cm$^{-1}$, respectively. Such a red shift in the spectral lines may be due to the substitution of one H atom in the pyridine ring with a CH$_3$ methyl group.

When comparing the experimentally obtained spectrum with the theoretically calculated spectrum, only small shifts in frequencies related to certain vibrations were observed. These discrepancies might be due to certain limitations in the theoretical calculations.

## CONCLUSION

The structure and vibrational properties of the 3-methylpyridine (C$_5$H$_4$N(CH$_3$)) molecule were investigated using Raman scattering and infrared absorption spectra, as well as theoretical calculations based on the Density Functional Theory (DFT) method and the (B3LYP) HF/6-311G$^{**}$ basis set. The contribution of the CH$_3$ group to the Raman spectrum was studied by comparing the 3-methylpyridine molecule to pyridine. It was noted that in the lower frequency range (100-1043 cm-1), the spectral line associated with the vibration of the pyridine ring shifted to higher frequencies, which is attributed to intermolecular H-bonding. The shift of the spectral lines formed by the rotational-twisting movements of the pyridine ring to lower frequencies was found to be related to the methyl substitution in the structure.

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