STUDY OF THE EFFECT OF BROMINE ATOMS IN THE O-DIBROMOBENZENE MOLECULE ON OPTICAL SPECTRA

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Abstract

The Raman scattering (RS) spectrum of light reflecting the laws of motion of the o-dibromobenzene molecule was studied in the frequency range of 100–3500 cm^1. Based on the experimental results and theoretical quantum-chemical calculations, it was suggested that the spectra formed at lower frequencies are related to the rotational-vibrational movement of the molecule, and the optical spectra in the higher frequency range are related to the rotational and vibrational movements.

Keywords: spectrum, Raman scattering, o-dibromobenzene, rotational-vibrational motion, frequency, polarizability.

The study of physical laws associated with relaxation processes occurring in condensed media under the influence of electromagnetic wave radiation is one of the problems of fundamental and practical importance. Based on the results of research, it is possible to obtain scientifically based information about the structure of the environment and make recommendations for practice.

This research work is a logical continuation of the work in this direction, and the o-dibromobenzene-$C_6H_4Br_2$ molecule, which has an asymmetric property in terms of the polarizability tensor, was chosen as the research object. o-dibromobenzene is a pale yellow, aromatic organic liquid. The chemical structure model of the molecule is represented in Fig.1. It can be seen from the picture that the o-dibromobenzene molecule is a product of the replacement of two hydrogen atoms in the benzene ring with bromine atoms, which is a halogen element.

Due to the fact that benzene and its derivatives have unique physical properties and are widely used in industry, many research studies have been conducted to study their structure. RS and IR absorption spectra of o-dibromobenzene liquid were analyzed using theoretical calculations [1]. In [2], dibromobenzenes (1,2-, 1,3- and 1,4-$C_6H_4Br_2$) were studied by theoretical calculations, and the geometric structure of the benzene ring was slightly disturbed due to the high electronegativity of bromine atoms.

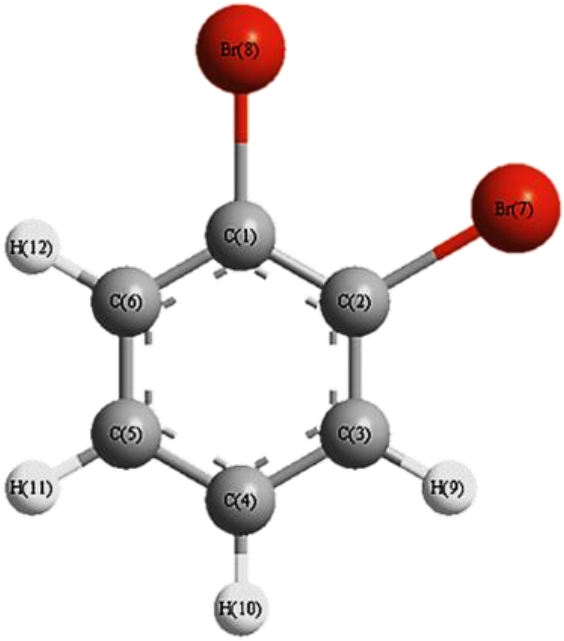

Fig.1. Chemical structural model of the o-dibromobenzene molecule

The RS spectra resulting from the vibrational and rotational motions of aromatic hydrocarbon molecules, which are asymmetric according to the polarizability tensor, were studied, and the mechanisms of optical spectra were studied [3,4].

Despite the fact that there is a lot of experimental data on the laws of various physical properties of benzene derivatives with halogen elements, currently there is no unified opinion about the processes that occur at the molecular level in these liquids. This situation means that these objects should be studied more widely.

Based on the above, this scientific research work is devoted to the study of the laws associated with the vibration and rotation of the o-dibromobenzene molecule using the experimentally obtained and quantum-chemically calculated RS method.

o-dibromobenzene was purchased from Sigma-Aldrich, a pure chemical reagent manufacturer in the United States. Its purity was 99.5% and was used in the experiment without further purification.

The RS spectrum was recorded on a spectrometer based on the InVia Raman spectrometer of the Renishaw company. Spectral resolution of Raman spectrometer is 0.3 cm^{-1}, spatial resolution is 0.25 μm. Laser radiation with a wavelength of 785 nm was used as a light source.

The experimentally obtained RS spectrum was recorded for the o-dibromobenzene molecule in the frequency range of 100–3500 cm^{-1}, and the frequency distribution of the spectrum is shown in Fig. 2-a.

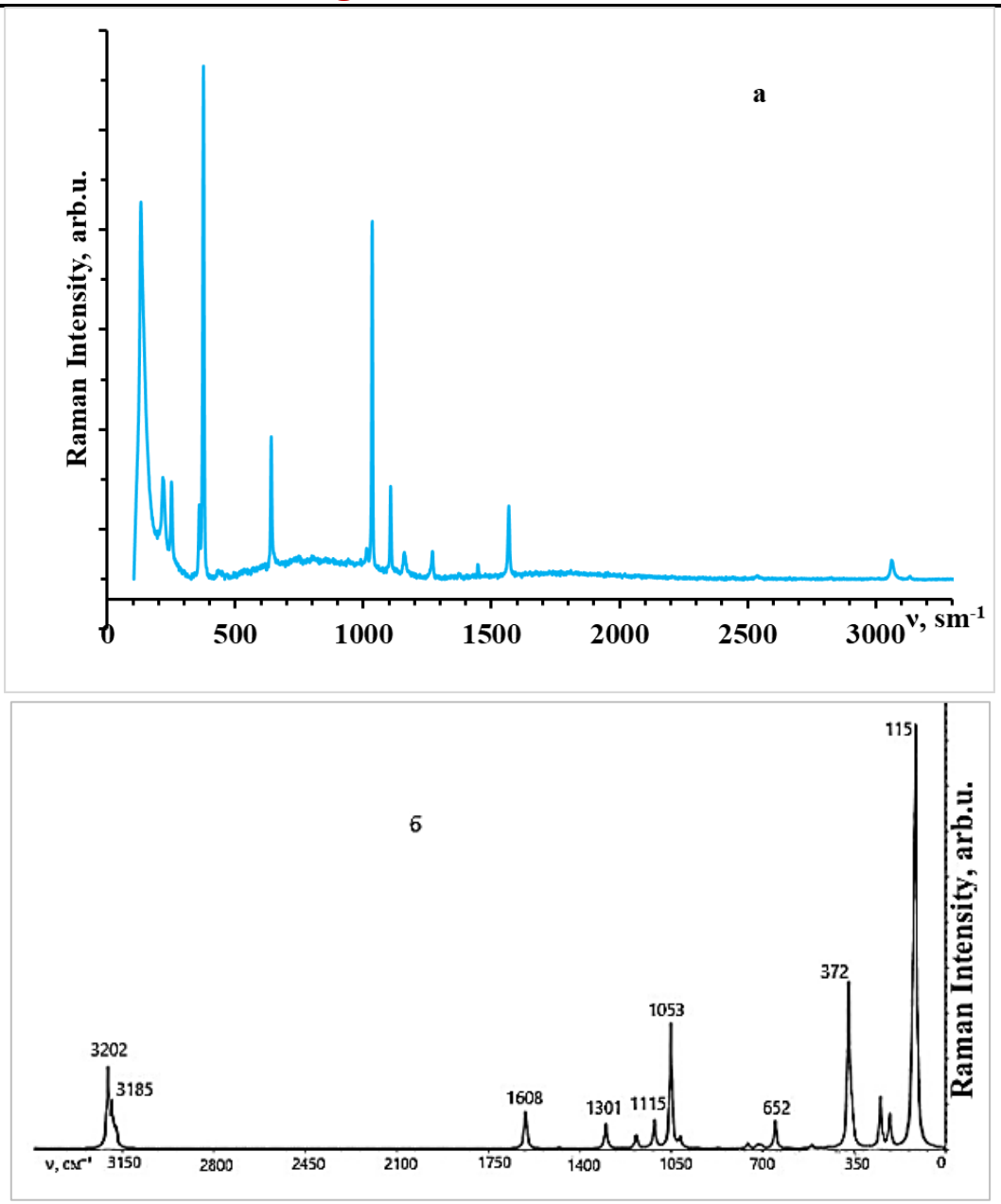

Fig.2. RS spectrum for the o-dibromobenzene molecule. a) experiment b) theoretical

The research results showed that 12 spectra with different intensities were observed in the frequency range of 100–3500 cm^{-1}. It was found that the formed spectra in the field of high frequencies are related to valence and deformation vibrations of the molecule.

The spectra in the lower frequency range appear as a result of the vibration of the molecule due to deformation, as well as the rotation-shaking movements of one part of the polyatomic molecule with a halide element (heavy atom) in its structure relative to another. It was determined that the spectral lines with frequency values of 375, 251, 220, and 131 cm^{-1} in the lower frequency range of

the RS spectrum belong to the in-plane and out-of-plane rotational movements of C-Br pairs, respectively. Corresponding to the low frequency range of the RS spectra formed by the rotation-reflection movements of atomic groups was also reflected in our previous scientific research conducted in other environments [3,4].

The overview of the theoretically calculated RS spectrum for the O-dibromobenzene molecule is shown in Fig. 2-b. Theoretical calculations were performed in the ORCA program, based on the Hartree-Fock method HF/6-311G** basis set. Typically, theoretically calculated frequency values are higher than the corresponding experimentally obtained frequency values due to electron correlation effects and Hartree-Fock basis set deficiencies. The total number of theoretically calculated spectra had the same result as the number of spectra obtained from the experiment.

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Adabiyotlar ro‘yxati

1. G. Shakila, S. Periandy, S. Ramalingam. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, V.86, 2012, P. 449-455.
2. Tsang-Hsiu Wang, Chen-Shuo Hsu, Wen-Lin Huang, Yih-Hsing Lo. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, V.115, 2013, P.866-875.
3. Dilafruz Khudoyberdieva, Shavkat Otajonov, Bakhodir Eshchanov, Husan Eshquvatov, Nuraddin Abdullayev, Mechanisms of Raman scattering spectrum of light from pyridine molecule in the lower frequency range, Results in Optics, 2024, 100685, ISSN 2666-9501. https://doi.org/10.1016/j.rio.2024.100685.
4. Ш. Отажонов, Б.Х. Эшчанов, Д.Б. Худойбердиева. O’zbekiston Respublikasi Fanlar akademiyasining ma’ruzalari, Toshkent 2023, №1, 24-28 betlar.