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# Study of the Molecular Composition of Gases by Molecular Spectroscopy and Quantum Chemical Calculations

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**Abstract:** Study of the molecular composition of gases by molecular spectroscopy and quantum chemical calculations. The study of any field of physics always begins with the introduction of a specific model, within which further research is carried out. For example, when we studied kinematics, the model of the body was a material point, when we studied the motion of the planets, the planets were spherical, and so on. As you might guess, the model never matches real processes, but often comes very close to matching.

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The study of any field of physics always begins with the introduction of a specific model, within which further research is carried out. For example, when we studied kinematics, the model of the body was a material point, when we studied the motion of the planets, the planets were spherical, and so on. As you might guess, the model never matches real processes, but often comes very close to matching.

Molecular physics and especially MKT are no exception. Since the 18th century, many scientists have worked on the problem of describing models: M. Lomonosov, D. Joule, R. Clausius (Fig. 1). The latter, in fact, introduced the ideal gas model in 1857.

Starting from the eighteenth century, he gradually began to form a system of scientific ideas about the structure of matter, called the molecular kinetic theory (MKT). Molecular Kinetic Theory generalizes the results of large-scale experimental data based on three experiments:

All bodies are made up of tiny particles - atoms, molecules and ions. Thus, any substance has a discrete structure.

The particles that make up matter are in constant chaotic motion, called thermal. Atoms, molecules and ions interact with each other. Please read these rules carefully.

Inert gases (helium, argon, etc.), liquids (mercury) and solids (copper, diamond) have a nuclear structure. A number of crystalline substances, such as sodium chloride, consist of oppositely charged ions. However, most substances are formed from molecules (carbon dioxide, water), so the term "molecule" is often used as a general collective term.

Modern experimental technique makes it possible to observe the molecular structure of a substance, as well as to determine the sizes of atoms and molecules. These dimensions are very small: for atoms they are up to  $10^{-10}$  m, and for molecules their range is much wider - from  $10^{-10}$  m for the simplest molecules to  $10^{-15}$  m for the molecules of complex organic substances.

Naturally, the mass of atoms and molecules with such dimensions is also very small, for

example, the mass of a hydrogen molecule is  $3.3 \cdot 10^{-27}$  kg. It is clear that in practical calculations it is not at all convenient to work with such a value.

Physical methods for studying the life of molecules.

We know from school courses in chemistry and physics that all substances are made up of atoms, molecules, ions, or combinations thereof. And we, like, even know what kind of life they live. But this information should have its own reliable sources (research methods), and they really do exist.

There are very, very many such ways to spy on the life of atoms. But, roughly and quite easily, 3 main groups of methods are distinguished:

1. spectroscopic methods,
2. diffraction methods,
3. various methods of microscopy (it doesn't matter whether it is translucent or scanning, it is not essential for us now).

There will be no talk about the last one, but its tools are no less important than those of the first two.

Spectroscopic methods for studying matter This powerful group of methods provides us with a lot, a lot: from finding and identifying molecules in the interstellar medium and on other planets to a banal check for explosives at an airport.

### **General principle of operation of spectral methods**

When people talk about spectroscopy, they usually mean the following general principle of operation.

We have something with which we (for example, a light bulb / laser / sunlight) affect the sample of interest to us. Most often this is an electromagnetic study, but this may well be electrons (for example, in mass spectroscopy with electron impact ionization) or a cocktail of everything possible and impossible from plasma (for example, in flame spectroscopy, so beloved by schoolchildren and undergraduate students of chemistry departments). One way or another, something must affect our sample.

When the sample is exposed to something, something happens that it changes its state. This can be a transition to some kind of excited level (in any spectrophotometry or Raman spectroscopy), or a general collapse of the molecular system (as in mass spectra or photoelectron spectroscopy). But one way or another, the pattern must be different at some point.

**PROFIT!!!** We register a certain signal (either emitted or absorbed) with this change in the sample at the molecular level. These can be lost photons spent on changing the sample (then we have absorption spectroscopy), or vice versa, extra photons emitted after the preliminary excitation of the substance (emission spectroscopy), a change in the wavelength of the initial photons as a result of interaction with the substance (Raman spectroscopy, more known abroad as Ramen's Raman), well, or stupidly fragments of primordial molecules (as in mass spectra or photoelectron spectroscopy). There are many options - the essence is the same: there is a signal!

Since in the vast majority of cases spectroscopy is still tied to electromagnetic radiation, it is logical to link the ranges of the electromagnetic spectrum to various aspects of atomic and molecular life. After all, the frequency of electromagnetic waves used in spectroscopy is a kind of "clock" that allows you to detect how long this or that process lasts in molecular

systems. So, by changing this frequency, you can study (and even influence) various molecular processes. So.

From a chemical point of view, nothing interesting happens in the ultra-longwave range, so you can forget about it.

With the frequency of radio and microwaves (and even long-wave infrared radiation, IR \u003d IR), different molecules rotate in the gas phase: large and heavy molecules in the radio wave region (lower frequencies), and small and light molecules in the IR region (higher frequencies).

➤ In IR, on the other hand, various vibrations of molecules (mostly) occur: all conformational and other non-obvious movements inside the molecules - in longwave IR, and stretching vibrations (stretching - shortening of the lengths of chemical bonds) - in short-wave (up to 4000  $\text{cm}^{-1}$ ).

A revision of the basic provisions of the quantum theory of the structure and properties of polyatomic molecules has been carried out. On the basis of the principle of mathematical representation of generally accepted models of polyatomic molecules, the main questions of setting quantum problems are considered.

Attention is drawn to the fact that, like the empirical formula, the Schrödinger equation adequate to it, which takes into account only the atomic composition of the compound and Coulomb interactions between electrons and nuclei, is not sufficient for concretizing the problem and does not allow one to single out, using only the "first principles" of quantum mechanics, the desired structural isomeric forms from their entire possible set (more than 106 for a system of 30 atoms).

A well-defined statement of the problem is possible if, starting from the structural formula and the corresponding adjacency matrix, we form an energy (Hamiltonian) matrix and use the matrix formulation of quantum mechanics. Such an approach is not the result of a search for an approximate solution of the Schrödinger differential equation. This is another self-sufficient formulation of the problem.

A new Schrödinger equation is proposed that is adequate to the mathematical representation of a molecular model in the form of a spatial figure with a certain arrangement of nuclei and taking into account their quantum "smearing". The localization of the motion of the nuclei is provided by a priori specification of the characteristics of the potential "well". The oscillatory wave function uniquely associated with it makes it possible to write the Schrödinger equations, which take into account the "smearing" of the nuclei, in separable variables - the coordinates of electrons and nuclei. The wave functions and eigenvalues of the electronic terms in such Hamiltonians automatically take into account the quantum characteristics of nuclear states. This has an analogy with the "soft" non-adiabatic approximation in traditional theory, but is more general. The approach makes it possible to take into account the peculiarities of nuclear motions not only within one "pit", but also in "pits" with two or more minima (inversion, cis-, trans-isomerism, internal rotation, etc.)

It is shown that with the help of sets of basic vibrational eigenfunctions for different sets of vibrational quantum numbers, it is possible to construct an energy matrix covering both all vibrational states of one isomeric form taken into account in the formulation of the problem, and several isomeric forms.

This allows further use of such a matrix not only to analyze the probabilities of optical transitions (spectra), but also nonradiative ones (chemical transformations). Expressions for all necessary matrix elements are found and methods for their calculation are indicated.

It is concluded that in the general quantum theory of the structure of molecules and molecular processes, the variants of quantum mechanics based on matrices (Heisenberg) and differential operators (Schrödinger) act not as equivalent, but as complementary (according to Bohr).

The whole new approach differs from the existing one in greater logical rigor and greater simplicity of calculations, which can be performed almost without changing the developed mathematical procedures.

The principal thing is the possibility of introducing a unified system of physically visual parameters (characteristics of the “well” of the ground state), which allow one to continuously influence vibrational and vibronic energy levels and wave functions.

This makes it possible to pose and solve various (spectral, etc.) inverse problems and refine the values of the electronic-vibrational energy levels and the characteristics of the wave functions, achieving good agreement with experiment. In the traditional theory, there are no such possibilities. Reliance directly on experimental data on IR and Raman spectra and molecular geometries and knowledge of their variations also creates the possibility of a priori estimation of the degree of reliability of the prediction of various calculated characteristics of molecules and more complex molecular formations.

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