

OPTICS AND SPECTROSCOPY

STUDY OF SPECTROSCOPIC PROPERTIES OF DIATOMIC MOLECULES BASED ON HIGH ORDERS OF THE OPERATOR PERTURBATION THEORY

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The form of the effective Hamiltonian of a quantum system with allowance for corrections of arbitrary order for solving arbitrary quantum-mechanical problems with perturbation operator depending not only on the same coordinates as the operator of the zero approximation, but also on an arbitrary set of other coordinates whose derivative operators may not commute with each other, is retrieved based on the operator perturbation theory (the recurrence formulas for corrections of any arbitrary order of the operator perturbation theory are presented in the paper in the most general form). The general results obtained allow the special features of the effective operators of any polyatomic molecule to be investigated. As a first step, an arbitrary diatomic molecule is investigated. Isotopic relations among different spectroscopic parameters are derived for the parent molecule and its various isotopic modifications.

Keywords: operator perturbation theory, diatomic molecules, isotopic relationships.

INTRODUCTION

One of the main problems of high-resolution spectroscopy is the determination of the fundamental properties of molecules of different types based on an analysis of their fine vibrational-rotational structure. Unfortunately, such analysis is complicated by the presence (especially for highly excited vibrational states) of numerous interactions (particularly, resonance ones) and effects. Moreover, an analysis of the modern high-resolution spectra suggests taking into account tens of thousands of experimental lines in models comprising hundreds of parameters. Under such conditions, the overwhelming majority of inverse spectroscopic problems to be solved are ill-posed. The most reasonable method of regularization of these problems is establishing as many relationships among the parameters as possible (for example, see [1–18]). In this case, the only method of solving this problem is to predict correctly positions of lines in the spectrum based on results of theoretical calculations of as many parameters of the employed model of the molecule as possible using the so-called *effective Hamiltonians* of the molecule [19–26].

In connection with the foregoing, a procedure for retrieving analytical relationships that allow the most important spectroscopic constants of a diatomic molecule to be related with the basic molecule parameters (including the intramolecular potential function parameters and the structural parameters of the molecule) and thereby interpretation of complex vibrational-rotational spectra for highly excited states to be greatly facilitated is considered in the present paper as a first step to a study of polyatomic molecules. The analysis is based on the matrix formulation of

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the operator perturbation theory [27–29]. The programming language *MAPLE* [30] was used for calculations because of their complexity. Isotopic relationships are considered for various spectroscopic parameters of diatomic molecules.

VIBRATIONAL-ROTATIONAL HAMILTONIAN OF A DIATOMIC MOLECULE AND THE OPERATOR PERTURBATION THEORY

Let us give the main formulas necessary for deriving relationships connecting the spectroscopic parameters with the basic parameters of a molecule. According to the vibrational-rotational theory [31, 32], the Hamiltonian of a diatomic molecule has the following form:

$$H = \frac{1}{2} P^2 + B \sum_{\alpha} J_{\alpha} + V, \quad (1)$$

$$B = B_e + b_1 q + b_2 q^2 + b_3 q^3 \dots, \quad (2)$$

$$V = \frac{(2\pi c)^2}{2} \omega^2 q^2 + k_3 q^3 + k_4 q^4 + k_5 q^5 + \dots, \quad (3)$$

where B is the rotational constant represented by Eq. (2), J_{α} are the components of the angular momentum operator, and V is the intramolecular potential function.

The main problem that researchers who would like to describe the state of a quantum system are facing is a solution of the Schrödinger equation. Knowledge of solutions of the Schrödinger equation allows the molecule to be investigated comprehensively as a quantum object. Indeed, the eigenvalues of the Hamiltonian retrieved from the solution of the Schrödinger equation are nothing else than the energies that can have the examined quantum system. Knowledge of the eigenfunctions allows the transition probabilities to be determined, and the average physical parameters characterizing the molecule to be calculated. However, it should be noted that an exact solution of the Schrödinger equation is possible only for the simplest molecular systems of the molecular ion of H^+ type. In the general case, it is impossible to obtain a solution of the Schrödinger equation. Therefore, various versions of the perturbation theory are used to solve these problems.

It can be shown (for example, see [33–38]) that the effective Hamiltonian of an arbitrary molecule can be written in the form

$$H_{\text{eff}} = \sum_{v, \tilde{v} \in \Omega} |v\rangle \langle \tilde{v}| H_{v\tilde{v}}, \quad (4)$$

$$H_{v\tilde{v}} = \sum_{n=0} H_{v\tilde{v}}^{(n)} (k^n), \quad (5)$$

where $|v\rangle$ and $|\tilde{v}\rangle$ are the vibrational functions belonging to a polyad of the interacting states, k is the small Born–Oppenheimer parameter, operators $H_{v\tilde{v}}$ depend only on the rotational operators J_{α} , and summation is performed over all degenerate and/or interacting vibrational states. In this case, due to the absence of a resonance interaction, Eq. (4) assumes the form

$$H_{\text{eff}}^v = |v\rangle \langle v| H_{vv}. \quad (6)$$

As shown in [29], the effective rotational operator $H_{v\tilde{v}}$ can be represented as

$$H_{vv} = \left\langle v \left| \sum_{k=0}^{\infty} \frac{1}{k!} \left[-i \sum_{n=1}^{\infty} g_n, H \right]^{(k)} \right| v \right\rangle. \quad (7)$$

The following notations have been used in Eq. (7):

$$[A, B]^{(0)} = B,$$

$$[A, B]^{(1)} = [A, B] = AB - BA, \quad (8)$$

$$[A, B]^{(2)} = [A, [A, B]].$$

The matrix elements of the operators ig_n ($n = 1, 2, \dots$) in Eq. (7), in their turn, are also derived based on the recurrence relationships

$$\langle v | ig_n | \tilde{v} \rangle = \frac{1}{E_v - E_{\tilde{v}}} \left\langle v \left| \sum_{r=0}^{\infty} \frac{1}{r!} \left[-i \sum_{l=1}^{\infty} ig_l, h \right]^{(r)} + \sum_{p=2}^{\infty} \frac{1}{p!} \left[-i \sum_{m=1}^{\infty} ig_m, H_0 \right]^{(p)} \right| \tilde{v} \right\rangle. \quad (9)$$

Equations (6)–(9) were used to determine the effective Hamiltonian of a diatomic molecule. In this case, the contributions up to the 5th order were taken into account. As an illustration, some of the $\langle v | ig_n | \tilde{v} \rangle$ operators and the form of the effective Hamiltonian $H_{\text{eff}}^{(5)}$ with corrections are presented below:

$$\langle v | ig_1 | v \rangle = \frac{H_{v\tilde{v}}}{\varepsilon_{\tilde{v}} - \varepsilon_v}, \quad (10)$$

$$\langle v | ig_2 | v \rangle = \sum_{\alpha \neq v, \alpha \neq \tilde{v}} \frac{h_{v\alpha} h_{\alpha\tilde{v}}}{2(\varepsilon_{\tilde{v}} - \varepsilon_v)} \left(\frac{1}{\varepsilon_v - \varepsilon_{\alpha}} + \frac{1}{\varepsilon_{\tilde{v}} - \varepsilon_{\alpha}} \right) + \frac{h_{v\tilde{v}}}{2(\varepsilon_{\tilde{v}} - \varepsilon_v)} (h_{vv} - h_{\tilde{v}\tilde{v}}), \quad (11)$$

$$\begin{aligned} H_{vv} = & \varepsilon + \langle v | h | v \rangle + \sum_{\alpha \neq v} \frac{\langle v | h | \alpha \rangle \langle \alpha | h | v \rangle}{(\varepsilon_v - \varepsilon_{\alpha})} + \dots - (\langle v | h | v \rangle)^3 \sum_{\alpha \neq v} \frac{\langle v | h | \alpha \rangle \langle \alpha | h | v \rangle}{(\varepsilon_v - \varepsilon_{\alpha})^4} \\ & + (\langle v | h | v \rangle)^2 \sum_{\alpha \neq v} \frac{\langle v | h | \alpha \rangle \langle \alpha | h | \beta \rangle \langle \beta | h | v \rangle}{(\varepsilon_v - \varepsilon_{\alpha})(\varepsilon_v - \varepsilon_{\beta})} \left\{ \frac{1}{(\varepsilon_v - \varepsilon_{\alpha})^2} + \frac{1}{(\varepsilon_v - \varepsilon_{\beta})^2} + \frac{1}{(\varepsilon_v - \varepsilon_{\alpha})(\varepsilon_v - \varepsilon_{\beta})} \right\} \\ & + \sum_{\substack{\alpha \neq v \\ \beta \neq v \\ \gamma \neq v \\ \delta \neq v}} \frac{\langle v | h | \alpha \rangle \langle \alpha | h | \beta \rangle \langle \beta | h | \gamma \rangle \langle \gamma | h | \delta \rangle \langle \delta | h | v \rangle}{(\varepsilon_v - \varepsilon_{\alpha})(\varepsilon_v - \varepsilon_{\beta})(\varepsilon_v - \varepsilon_{\gamma})(\varepsilon_v - \varepsilon_{\delta})} \\ & + \sum_{\substack{\alpha \neq v \\ \beta \neq v}} \frac{\langle v | h | \alpha \rangle \langle \alpha | h | v \rangle \langle v | h | \beta \rangle \langle \beta | h | v \rangle \langle v | h | v \rangle}{(\varepsilon_v - \varepsilon_{\alpha})(\varepsilon_v - \varepsilon_{\beta})} \left\{ \frac{1}{(\varepsilon_v - \varepsilon_{\alpha})^2} + \frac{1}{(\varepsilon_v - \varepsilon_{\beta})^2} + \frac{1}{(\varepsilon_v - \varepsilon_{\alpha})(\varepsilon_v - \varepsilon_{\beta})} \right\} \quad (12) \end{aligned}$$

$$\begin{aligned}
& - \sum_{\substack{\alpha \neq \nu \\ \beta \neq \nu \\ \gamma \neq \nu}} \frac{\langle \nu | h | \alpha \rangle \langle \alpha | h | \nu \rangle \langle \nu | h | \beta \rangle \langle \beta | h | \gamma \rangle \langle \gamma | h | \nu \rangle}{(\varepsilon_\nu - \varepsilon_\alpha)(\varepsilon_\nu - \varepsilon_\beta)(\varepsilon_\nu - \varepsilon_\gamma)} \left\{ \frac{1}{(\varepsilon_\nu - \varepsilon_\alpha)} + \frac{1}{(\varepsilon_\nu - \varepsilon_\beta)} + \frac{1}{(\varepsilon_\nu - \varepsilon_\gamma)} \right\} \\
& - \sum_{\substack{\alpha \neq \nu \\ \beta \neq \nu \\ \gamma \neq \nu}} \frac{\langle \nu | h | \alpha \rangle \langle \alpha | h | \beta \rangle \langle \beta | h | \gamma \rangle \langle \gamma | h | \nu \rangle \langle \nu | h | \nu \rangle}{(\varepsilon_\nu - \varepsilon_\alpha)(\varepsilon_\nu - \varepsilon_\beta)(\varepsilon_\nu - \varepsilon_\gamma)} \left\{ \frac{1}{(\varepsilon_\nu - \varepsilon_\alpha)} + \frac{1}{(\varepsilon_\nu - \varepsilon_\beta)} + \frac{1}{(\varepsilon_\nu - \varepsilon_\gamma)} \right\} + \dots
\end{aligned}$$

SPECTROSCOPIC CONSTANTS FOR A DIATOMIC MOLECULE

It is well known that the energy of a diatomic molecule is determined by the formula

$$E(v, J) = \sum_{i,j} Y_{ij} \left(v + \frac{1}{2} \right)^i [J(J+1)]^j, \quad (13)$$

where Y_{ij} are the spectroscopic parameters (frequencies, anharmonic frequencies, rotational and centrifugal constants, etc.):

$$\begin{aligned}
Y_{10} &= \omega, \quad Y_{20} = x, \quad Y_{30} = y, \dots \\
Y_{01} &= B_e, \quad Y_{11} = \alpha, \quad Y_{21} = \beta, \dots \\
Y_{02} &= D_e.
\end{aligned} \quad (14)$$

Using the perturbation theory, it can be shown that E, B, Δ , and H_e have the following form:

$$E = E_0 + x \left(v + \frac{1}{2} \right)^2 + y \left(v + \frac{1}{2} \right)^3 + z \left(v + \frac{1}{2} \right)^4 + \dots, \quad (15)$$

$$B = B_e + \alpha \left(v + \frac{1}{2} \right) + \gamma \left(v + \frac{1}{2} \right)^2 + \delta \left(v + \frac{1}{2} \right)^3 + \dots, \quad (16)$$

$$\Delta = \Delta_e + \Delta_1 \left(v + \frac{1}{2} \right) + \Delta_2 \left(v + \frac{1}{2} \right)^2 + \dots, \quad (17)$$

$$H = H_e + H_1 \left(v + \frac{1}{2} \right) + \dots \quad (18)$$

Direct substitution of Eqs. (1)–(3) into general formulas (10)–(18) makes it possible to obtain different Y_{ij} parameters as functions of the parameters ω, K_n, B_e , and α_m . As an illustration, we present some results that allow in principle predictive calculations to be performed and parameters of the intramolecular potential function to be determined based on the experimental vibrational-rotational spectra of the molecule:

$$Y_{10} = \frac{25k_6}{8} - \frac{67k_4^2}{16\omega} - \frac{95k_3k_5}{8\omega} + \frac{459k_3^2k_4}{16\omega^2} - \frac{1155k_3^4}{64\omega^3},$$

TABLE 1. Values of the Spectroscopic Parameters Y_{02} and Y_{03}

Molecule	Y_{02} (theor.)	Y_{02} (exp.)	Y_{03} (theor.)	Y_{03} (exp.)
HCl ³⁵	$-5.315427 \cdot 10^{-4}$	$-5.318961 \cdot 10^{-4}$	$1.700 \cdot 10^{-8}$	$1.737 \cdot 10^{-8}$
HCl ³⁷	$-5.299364 \cdot 10^{-4}$	$-5.297529 \cdot 10^{-4}$	$1.68685 \cdot 10^{-8}$	$1.5852 \cdot 10^{-8}$
DCI ³⁵	$-1.406202 \cdot 10^{-4}$	$-1.404857 \cdot 10^{-4}$	$2.30685 \cdot 10^{-9}$	$1.5108 \cdot 10^{-9}$
DCI ³⁷	$-1.397894 \cdot 10^{-4}$	$-1.396645 \cdot 10^{-4}$	$2.28607 \cdot 10^{-9}$	$1.8078 \cdot 10^{-9}$
TCI ³⁵	$-6.6150 \cdot 10^{-5}$	$-6.6090 \cdot 10^{-5}$	$7.442 \cdot 10^{-10}$	$4.875 \cdot 10^{-10}$

$$\begin{aligned}
 Y_{20} = & \frac{3k_4}{2} + \frac{245k_6}{16} - \frac{15k_3^2}{4\omega} - \frac{1365k_3k_7}{16\omega} - \frac{885k_4k_6}{16\omega} - \frac{1085k_5^2}{32\omega} + \frac{8535k_3^2k_6}{32\omega^2} + \frac{7335k_3k_4k_5}{16\omega^2} + \frac{1707k_4^3}{32\omega^2} \\
 & - \frac{23865k_3^3k_5}{32\omega^3} - \frac{62013k_3^2k_4^2}{64\omega^3}, \\
 Y_{30} = & \frac{5k_6}{2} - \frac{17k_4^2}{4\omega} - \frac{35k_3k_5}{2\omega} + \frac{225k_3^2k_4}{4\omega^2} - \frac{705k_3^4}{16\omega^3} - \frac{705k_3^4}{16\omega^3}, \\
 Y_{01} = & 1 - \frac{15k_5b_1}{8\omega} - \frac{7k_3b_3}{8\omega} - \frac{3k_4b_2}{4\omega} + \frac{23b_1k_3k_4}{4\omega^2} + \frac{7k_3^2b_2}{4\omega^2} - \frac{21b_1k_3^3}{4\omega^3}.
 \end{aligned}$$

To illustrate the correctness of the results obtained, numerical test calculations of the coefficients Y_{02} and Y_{03} were carried out. It should be noted that Y_{03} depends on the parameter k_3 of the potential function. To determine this parameter, experimental values of the vibrational-rotational coefficient Y_{11} were used. The spectroscopic parameter values found from the theoretical prediction using the relationships obtained are given in Table 1. For a comparison, the values of these parameters taken from experimental data are also presented in Table 1. A more than satisfactory agreement between the calculated and experimental data for the parameter Y_{02} can be seen for all molecules without exception (the errors were of the order of 0.1%). The agreement with the experiment for the parameters Y_{03} was slightly worse. The difference between the prediction and experiment was mainly within 3–4%, but in some cases (as can be seen from Table. 1, for molecules containing deuterium and tritium) the difference reached a few tens of percent. We believe that the reason is the imperfection of the experimental data for these molecules.

ISOTOPIC RELATIONSHIPS FOR THE SPECTROSCOPIC PARAMETERS

It is well known that the application of the isotopic effect is a highly efficient method for a study of the vibrational-rotational spectra of molecules (for example, see [39–42]). Expressions obtained for the parameters of the Hamiltonian of a diatomic molecule, as shown above, are functions of the rotational constants, harmonic frequencies, and parameters of the intramolecular potential function, but the coordinates introduced above are not isotopically invariant. Therefore, to use the model for simultaneous consideration of several isotopic modifications, the model must be modified a little using an isotopically invariant set of coordinates (for example, see [43–45]), in our case, the natural vibrational coordinates. In these coordinates, the potential function in the Born–Oppenheimer approximation used for our analysis is independent of masses and hence, the parameters of the potential function f_n are the same for any isotopic modification of the molecule. For a diatomic molecule, the potential function in the natural coordinates can be taken in the form

$$V = \sum_n \frac{1}{n!} f_n \Delta r^n. \quad (19)$$

The parameters k_n were derived from Eq. (3) based on Eq. (19) using the analytic programming language *MARPLE* as functions of the parameters of the intramolecular potential function f_n :

$$k_3 = \frac{\sqrt{2}}{3} \left(\frac{B_e}{\omega} \right)^3 \left(\frac{f_3 \rho^3}{2\pi c \hbar} \right), \quad (20)$$

$$k_4 = \frac{2}{9} \left(\frac{B_e}{\omega} \right)^2 \left(\frac{f_4 \rho^4}{2\pi c \hbar} \right), \quad (21)$$

$$k_5 = \frac{\sqrt{2}}{30} \left(\frac{B_e}{\omega} \right)^5 \left(\frac{f_5 \rho^5}{2\pi c \hbar} \right), \quad (22)$$

$$k_6 = \frac{1}{90} \left(\frac{B_e}{\omega} \right)^3 \left(\frac{f_6 \rho^6}{2\pi c \hbar} \right), \quad (23)$$

where $B_e = \frac{\hbar}{4\pi c \rho^2 \mu}$, $\mu = \frac{m_1 m_2}{m_1 + m_2}$, and $\omega = \frac{\left(\frac{f_2}{\mu} \right)^{\frac{1}{2}}}{2\pi c}$.

Taking into account Eqs. (21)–(23) and relationships for the spectroscopic parameters Y_{ij} derived above, the following general relationships between the arbitrary parameters of the parent and isotopically substituted molecules can be derived:

$$Y'_{ij} = \left(\frac{\mu}{\mu'} \right)^{\frac{i}{2}+j} Y_{ij}. \quad (24)$$

To illustrate the correctness of Eq. (24), Table 2 presents values of the indicated spectroscopic parameters of diatomic molecules calculated by Eq. (24) and, for a comparison, the corresponding experimental data borrowed from [46–49]. A more than satisfactory agreement between both sets of values can be seen.

It should be noted that the diatomic molecules have only one vibrational degree of freedom and hence, are a good *touchstone* for testing the general approaches supposed to be used in nearest future for a study of much more complex polyatomic molecules.

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TABLE 2. Values $\frac{Y'_{ij}}{Y_{ij}}$ for the Indicated Diatomic Molecules

ij	$\frac{\text{HCl}^{35}}{\text{DCl}^{37}}$		$\frac{\text{HCl}^{35}}{\text{TCI}^{37}}$		$\frac{\text{HF}}{\text{DF}}$		$\frac{\text{HF}}{\text{TF}}$	
	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.
10	0.7158	0.7161	0.5919	0.5939	0.7245	0.7249	0.6055	0.6063
20	0.5123	0.5131	0.3503	0.3527	0.5250	0.5255	0.3666	0.3676
01	0.5123	0.5128	0.3503	0.3527	0.5250	0.5254	0.3666	0.3676
11	0.3667	0.3672	0.2073	0.2095	0.3804	0.3808	0.2220	0.2227
21	0.2625	0.2626	0.1227	0.1239	0.2756	0.2758	0.1344	0.1349
02	0.2625	0.2625	0.1227	0.1242	0.2756	0.2761	0.1344	0.1351
12	0.1879	0.1864	0.0726	0.0727	0.1997	0.1938	0.0814	0.0793

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