Scientific Research

# Determination of the Vibro-Rotational Constants, the Dipole Moment's Function and the Intensities of the HTO's $v_1$ ($v_3$ by Usual Convention) Band

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## ABSTRACT

In the first part of this paper, an analysis of the high-resolution spectrum of the HTO molecule $v_1(v_3)$ band, from 3630 to 3950 cm$^{-1}$, was undertaken. The rotational transition of this band was assigned using combination differences. Their wavenumbers were analyzed with a least squares fit program in order to obtain spectroscopic constants. A perturbed state has been evidenced. In the second part, with a view towards building a spectroscopic data base, a calculation of the dipolar momentum function was undertaken.

## 1. Introduction

HTO molecule is important for the environment. It is found in discharges of nuclear power plants with 12.3 years for half-life. It is essential to know its infrared spectrum in order to detect it remotely. It is also interesting to have available database to use this molecule spectroscopy. These were the motivation of our work focused on the fundamental $v_1(v_3)$ looks near 3700 cm$^{-1}$. The aim of this paper is twofold, firstly we perform a comprehensive analysis of high-resolution spectrum of the $v_1(v_3)$ band, and secondly we determine the dipole moment's function which will permit us to calculate the rays intensities in a wide range of quantum numbers.

We continued with an analysis of the transitions wave numbers to determine the spectroscopic constants that are essential to calculate the positions of such transitions.

## 2. Theoretical Calculations

### 2.1. The Vibration-Rotation Hamiltonian

Leaving from the approximations of Born Oppenheimer [1,2] and of the harmonic that consists in separating the movement of the electrons to that of the cores and in describing the molecule while developing only the potential energy to the second order, with the help of the 3N-6 correctly chosen coordinates. The vibration-rotation Hamiltonian, under compact shape, is written, according to Darling and Dennison [3], simplified by Watson [4,5],

by:

$$H = \frac{1}{2}\sum_{\alpha\beta}\left(J_\alpha - P_\alpha\right)\mu_{\alpha\beta}\left(J_\beta - P_\beta\right)$$
$$+ \frac{1}{2}\sum_{k=1}P_k^2 + V(Q) + U(Q) \tag{1}$$

where the indices $\alpha$ and $\beta$ correspond to the *xyz* axes of the mobile reference mark. $J_\alpha$ and $p_\alpha$ quantities are respectively the components of the total angular moment and the internal angular moment of the vibration; $\mu_{\alpha\beta}$ represents the component of the efficient inertia tensor's inverse; $p_k$ with $1 \le K \le 3N-6$ the conjugated momentum of the normal coordinate of $Q_k$ vibration; $V(Q)$ the potential energy (quadratic) and $U(Q)$ a term of a potential energy type. For the zero-order this Equation (1) becomes:

$$H_0 = H_v + H_r$$

With

$$H_v = \frac{1}{2}\sum_{k=1}^{3}\left(P_k^2 + \lambda Q_k^2\right) \tag{2}$$

By introducing the dimensionless normal coordinates, we obtain:

$$q_k = \frac{\lambda_k^{1/4}}{\hbar^{1/2}}Q_k \quad \text{and} \quad p_k = \frac{-i\partial}{\partial q_k}$$

The Equation (2) gets under the shape:

$$H_v = hc\sum_{k=1}^{3}\frac{\omega_k}{2}\left(p_k^2 + q_k^2\right) \tag{3}$$

where $\omega_k = \dfrac{\lambda_k^{1/2}}{2\pi c}$ is the $k$ node energy in cm$^{-1}$ and the $c$ constant, the light speed. The Equation (3) is the sum of three harmonic oscillators. We deduce easily the wave's function as well as the vibrational energy:

$$\Psi_v\left(v_1, v_2, v_3\right) = \prod_{k=1}^{3} \Phi_{vk}\left(q_k\right)$$

and

$$E_v = hc\sum_{k=1}^{3} \omega\left(v_k + \frac{1}{2}\right) \tag{4}$$

where $\Phi_v(q)$ is the harmonic oscillator wave's function for the vibrational quantum number $v$. From this equation, the values of the H$_2$O, HDO and HTO three normal nodes energies are given in the **Table 1**. The calculation has been done taking into account the molecule geometry at the equilibrium state and the surface potential energy of Patridge and Schwenke [6]. To compare our results, some energy levels, coming from the results of the references [7-12], were presented in the same table. We represented the small displacements to the H$_2$O isitopic in **Figure 1**. The normal modes are labeled using the IUPAC convention [13], followed in brackets by the usual convention. $H_r$ can be written by:

$$H_r = \sum_\alpha B_\alpha J_\alpha^2 \tag{5}$$

where $\alpha$ corresponds to the $x$, $y$, $z$ axes and

$$B_\alpha\left(\text{cm}^{-1}\right) = \frac{h}{8\pi^2 c}\frac{1}{I_\alpha^e}$$

$H_r$ has been calculated choosing the reference related to the $O'xyz$ molecule while the tensor of inertia would be diagonal (**Figure 2**).

For an asymmetric molecule type, as HTO, the use is to designate by $A$, $B$ and $C$ the constants of the rotational $B_\alpha$, with $A > B > C$. The corresponding axes have been noted $a$, $b$, $c$.

**Table 1. Calculated and observed energies of the three normal modes for the isotopic varieties of water.**

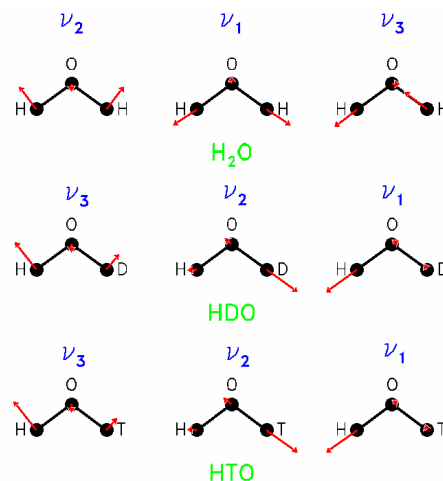| Variety | Mode | Calculated | Observed |
|---|---|---|---|
| | $v_1$ | 3831 | 3655 |
| H$_2$O | $v_2$ | 1648 | 1594 |
| | $v_3$ | 3942 | 3755 |
| | $v_1$ | 3889 | 3707 |
| HDO | $v_2$ | 2824 | 2726 |
| | $v_3$ | 1445 | 1403 |
| | $v_1$ | 3888 | 3716 |
| HTO | $v_2$ | 2369 | 1648 |
| | $v_3$ | 1370 | 1332 |



**Figure 1. The small displacements of the three normal nodes of vibration [13] of H$_2$O, HDO and HTO.**
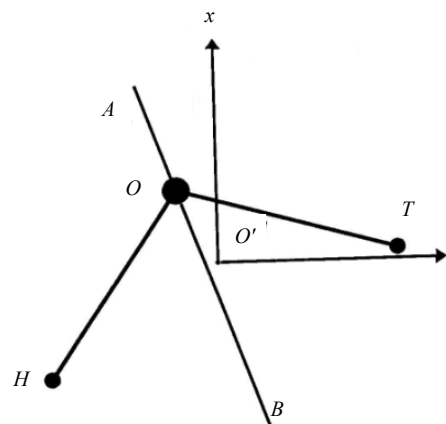


**Figure 2. The axes systems of HTO molecule.**

Following the $I^r$ representation $\left(x = b, y = c, z = a\right)$ the Equation (5) becomes :

$$\begin{aligned}
H_r &= AJ_z^2 + BJ_x^2 + CJ_y^2 \\
&= \left[A - \frac{1}{2}(B+C)\right]J_z^2 + \frac{1}{2}(B+C)J^2 \\
&\quad + \frac{1}{4}(B-C)\left(J_+^2 + J_-^2\right)
\end{aligned} \tag{6}$$

where $J^2 = J_x^2 + J_y^2 + J_z^2$ and $J\pm = J_x \pm iJ_y$.

To estimate the molecule's asymetry, we introduce the Ray parameter [14] $\kappa$, equal to $-0.8$. This means that the HTO molecule is enough close to a stretching asymmetric rotator ($\kappa = -1$).

There is no analytical forms for the eigenvalues of the Equation (5). To obtain the rotation energy, it is necessary to diagonalize the matrix of this hamiltonian in the basis $\left|J, K, M\right\rangle$ of the simultaneous eigenstates of the total angular momentum $J^2$ and of its projections on the laboratory $Z$ axis and the variable $z$ of the mobile reference, respectively, $J_Z$ and $J_z$.

$$J^2\left|J,K,M\right\rangle = J\left(J+1\right)\left|J,K,M\right\rangle$$
$$J_Z\left|J,K,M\right\rangle = M\left|J,K,M\right\rangle \qquad (7)$$
$$J_z\left|J,K,M\right\rangle = K\left|J,K,M\right\rangle$$

where $J$, $K$, $M$ is the quantum numbers corresponding to these three operators. The expression of the wave function $\left|J,K,M\right\rangle$ depends on the chosen conventions. In the present case we take the same convention of Bunker [15] and we write it as the following way:

$$\left|J,K,M\right\rangle = \sqrt{\frac{2J+1}{8\pi^2}} D_{KM}^{(J)}\left(\chi,\theta,\phi\right) \qquad (8)$$

where

$$D_{KM}^{(J)}\left(\chi,\theta,\phi\right) = e^{iK\chi} d_{KM}^{(J)}\left(\theta\right) e^{iK\phi}$$

The function $d_{KM}^{(J)}$ is defined in the reference [16]. When the molecule is isolated, the rotational energy doesn't depend on $M$ and, to simplify, we use the linear combinations of the following $\left|J,K\right\rangle$ functions:

$$\left|J,K,\gamma\right\rangle = \begin{cases} \dfrac{\left|J,K\right\rangle + \gamma\left|J,-K\right\rangle}{\sqrt{2}} & \text{for } K>0 \\[2mm] \left|J,K=0\right\rangle & \text{for } K=0 \end{cases} \qquad (9)$$

where $\gamma = \pm 1$. When $K=0$, only the linear combination with $\gamma = +1$ exists. The non zero matrix elements of the rotational Hamiltonian (Equation (5)), could exist only when the linear combinations and the Equation (9) are in the same type. That means $\Delta K = 0, \pm 2$ and $\Delta\gamma = 0$. We can write the rotational Hamiltonian eigenfunctions as followed:

$$\Psi_v^n = \sum_K a_{K,\gamma}^n \left|J,K,\gamma\right\rangle \qquad (10)$$

where $n$ is a quantum number varying from 0 to $2J$ and where $a_{K,\gamma}^n$ the related coefficients of the developing wave's functions. Rather than to use the quantum number $n$ to identify the rotation levels, we prefer to use the pseudo quantum numbers $K_a$ and $K_c$ of the rotation [17]. Although these latters are not real quantum numbers, all of the three quantum numbers $J$, $K_a$ and $K_c$ with $0 \le K_a \le J$, $0 \le K_c \le J$ and

$$K_a + K_c = J \text{ or } = J+1 \qquad (11)$$

permit to, unequivocally, identify the $2J+1$ rotation levels corresponding to a value of $J$. Indeed, we have $n = J + K_a + K_c$.

$E_r$ the rotation energy of the $J$, $K_a$, $K_c$ level, we can write:

$$H_r \Psi_r^{J,K_a,K_c} = E_r \Psi_r^{J,K_a,K_c} \qquad (12)$$

The **Figure 3** shows the arrangement of first levels of rotation of HTO. We will notice that the energy especially depends on $J$ and $K_a$. Two levels, character-
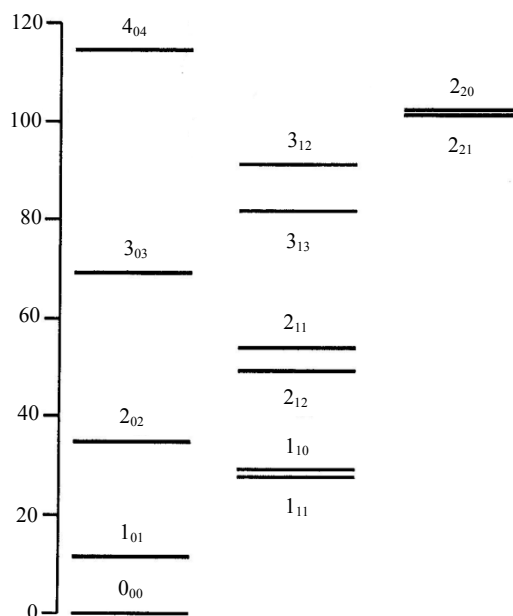


**Figure 3. Diagram of rotations energies levels of HTO.**

ized by the same values of these two quantum numbers with different $K_c$ values, have slightly different energies because of the asymmetry duplication. This latter increases with $J$ but decreases with $K_a$ and it is resulting from the fact that $B \ne C$. So the Hamiltonian of zero-order becomes:

$$\Psi_0 = \left|v_1,v_2,v_3,J,K_a,K_c\right\rangle = \Psi_r^{v_1,v_2,v_3}\Psi_r^{J,K_a,K_c} \qquad (13)$$

### 2.1.1. Watson's Hamiltonian

The above given results are only valid in the setting of the zero order approximation. In order to consider the centrifugal distortion effects, we will use the Watson's Hamiltonian [18-20]. However in this equation the rotational energy is not the eigenvalue of the rotational Hamiltonian of the Equation (6) but the eigenvalue of the efficient Hamiltonian depending only on the angular momentum of the rotation.

$$\begin{aligned}
H_r =\ & A^v J_z^2 + B^v J_x^2 + C^v J_y^2 - \Delta_K^v J_z^4 - \Delta_{KJ}^v J^2 J_z^2 - \Delta_J^v J^4 \\
& - \left\{\delta_K^v J_z^2 + \delta_J^v J^2, J_{xy}^2\right\} + H_K^v J_z^6 + H_{KJ}^v J^2 J_z^4 + H_{JK}^v J^4 J_z^2 \\
& + H_J^v J^6 + \left\{h_K^v J_z^4 + h_{KJ}^v J^2 J_z^2 + h_J^v J^4, J_{xy}^2\right\} + L_K^v J_z^8 \\
& + L_{KKJ}^v J^2 J_z^6 + L_{KJ}^v J^4 J_z^4 + L_{KJJ}^v J^6 J_z^2 + L_J^v J^8 \\
& + \left\{l_K^v J_z^6 + l_{KJ}^v J^2 J_z^4 + l_{JK}^v J^4 J_z^2 + l_J^v J^6, J_{xy}^2\right\} \\
& + P_K^v J_z^{10} + P_{KKKKJ}^v J^2 J_z^8 + P_{KKJ}^v J^4 J_z^6 + P_{KJJ}^v J^6 J_z^4 \\
& + P_{KJJJ}^v J^8 J_z^2 + P_J^v J^{10} \\
& + \left\{p_K^v J_z^8 + p_{KKJ}^v J^2 J_z^6 + p_{KJ}^v J^4 J_z^4 + p_{KJJ}^v J^6 J_z^2 + p_J^v J^8, J_{xy}^2\right\} \\
& + \cdots
\end{aligned}$$

$$(14)$$

where $J_{xy}^2 = J_x^2 - J_y^2$ and $\{,\}$ is the ant-commutator as $\{A,B\} = AB + BA$ .

In this equation, all parameters depend on the considered vibrationnal state as indicated by the exhibitor *v*. The adopted resolution is the A-type which is more adequate for an asymmetric molecule as HTO.

390 transitions have been assigned for *J* values below 15 (**Table 2**).

## 2.1.2. The Wave Numbers

For every transition, characterized by the rotationnal quantum numbers $J', K_a', K_c'$ and $J'', K_a'', K_c''$ for the lower and higher levels, respectively, the wave number $\sigma^{cal}$ has been calculated by:

$$\sigma^{cal} = E_r\left(J', K_a', K_c' : P^1\right) - E_r\left(J'', K_a'', K_c'' : P^0\right) + E_v^1 - E_v^0 \tag{15}$$

**Table 2. The transitions assigned in the infrared spectrum of the $v_1(v_3)$ band of HTO.**

| $J'$ | $K_a'$ | $K_c'$ | $J''$ | $K_a''$ | $K_c''$ | Obs | Cal | Diff |
|---|---|---|---|---|---|---|---|---|
| 2 | 2 | 1 | 3 | 2 | 2 | 3678.521(10) | 3721.521 | −43 |
| 1 | 0 | 1 | 2 | 1 | 2 | 3678.849(10) | 3658.849 | 20 |
| 6 | 1 | 6 | 6 | 1 | 5 | 3680.963(10) | 3692.963 | −12 |
| 3 | 1 | 3 | 4 | 0 | 4 | 3682.342(10) | 3704.342 | −22 |
| 2 | 1 | 2 | 3 | 1 | 3 | 3683.105(10) | 3696.105 | −13 |
| 5 | 0 | 5 | 5 | 1 | 4 | 3683.710(10) | 3669.710 | 14 |
| 5 | 2 | 4 | 4 | 3 | 1 | 3686.775(10) | 3549.775 | 137* |
| 0 | 0 | 0 | 1 | 1 | 1 | 3688.956(10) | 3660.956 | 28 |
| 4 | 0 | 4 | 4 | 1 | 3 | 3689.717(10) | 3687.717 | 2 |
| 5 | 1 | 5 | 5 | 1 | 4 | 3690.777(10) | 3698.777 | −8 |
| 5 | 2 | 3 | 4 | 3 | 2 | 3690.777(50) | 3714.777 | −24 |
| 1 | 1 | 0 | 2 | 1 | 1 | 3690.937(10) | 3693.937 | −3 |
| 8 | 2 | 7 | 8 | 2 | 6 | 3691.777(10) | 4057.777 | −362* |
| 1 | 0 | 1 | 2 | 0 | 2 | 3693.354(10) | 3679.354 | 14 |
| 4 | 2 | 3 | 5 | 1 | 4 | 3693.994(10) | 3603.994 | 90* |
| 1 | 1 | 1 | 2 | 1 | 2 | 3694.065(50) | 3688.065 | 6 |
| 3 | 0 | 3 | 3 | 1 | 2 | 3694.102(10) | 3686.102 | 8 |
| 3 | 1 | 3 | 2 | 2 | 0 | 3694.970(10) | 3694.970 | 0 |
| 2 | 1 | 2 | 3 | 0 | 3 | 3695.623(10) | 3695.623 | 0 |
| 11 | 5 | 7 | 11 | 5 | 6 | 3696.543(10) | 3678.543 | 18 |
| 11 | 5 | 6 | 11 | 5 | 7 | 3696.643(10) | 3680.643 | 16 |
| 2 | 0 | 2 | 2 | 1 | 1 | 3697.093(10) | 3680.093 | 17 |
| 6 | 2 | 5 | 5 | 3 | 2 | 3697.172(10) | 3392.172 | 305* |
| 10 | 5 | 6 | 10 | 5 | 5 | 3697.518(10) | 3665.518 | 32 |
| 10 | 5 | 5 | 10 | 5 | 6 | 3697.518(10) | 3703.518 | −6 |
| 10 | 6 | 5 | 10 | 6 | 4 | 3697.708(10) | 3714.708 | −17 |
| 10 | 6 | 4 | 10 | 6 | 5 | 3697.708(10) | 3715.708 | −18 |
| 9 | 6 | 4 | 9 | 6 | 3 | 3698.242(10) | 3655.242 | 43 |
| 9 | 6 | 3 | 9 | 6 | 4 | 3698.242(10) | 3655.242 | 43 |
| 9 | 5 | 5 | 9 | 5 | 4 | 3698.360(10) | 3693.360 | 5 |
| 9 | 5 | 5 | 9 | 5 | 5 | 3698.360(10) | 3703.360 | −5 |
| 8 | 6 | 3 | 8 | 6 | 2 | 3698.658(10) | 3719.658 | −21 |
| 8 | 6 | 2 | 8 | 6 | 3 | 3698.658(10) | 3719.658 | −21 |
| 1 | 0 | 1 | 1 | 1 | 0 | 3698.941(10) | 3665.941 | 33 |
| 8 | 5 | 4 | 8 | 5 | 3 | 3699.149(10) | 3699.149 | 0 |
| 8 | 5 | 3 | 8 | 5 | 4 | 3699.149(10) | 3702.149 | −3 |
| 6 | 6 | 0 | 6 | 6 | 1 | 3699.524(10) | 3702.524 | −3 |
| 6 | 6 | 1 | 6 | 6 | 0 | 3699.524(10) | 3702.524 | −3 |
| 6 | 5 | 1 | 6 | 5 | 2 | 3700.508(10) | 3697.508 | 3 |
| 6 | 5 | 2 | 6 | 5 | 1 | 3700.508(10) | 3697.508 | 3 |
| 5 | 5 | 0 | 5 | 5 | 1 | 3701.061(10) | 3694.061 | 7 |
| 5 | 5 | 1 | 5 | 5 | 0 | 3701.061(10) | 3694.061 | 7 |
| 4 | 1 | 4 | 3 | 2 | 1 | 3702.410(50) | 3694.410 | 8 |
| 9 | 3 | 7 | 9 | 3 | 6 | 3702.935(10) | 3718.935 | −16 |
| 9 | 4 | 5 | 9 | 4 | 6 | 3702.935(10) | 3664.935 | 38 |
| 8 | 4 | 5 | 8 | 4 | 4 | 3703.183(10) | 3699.183 | 4 |
| 7 | 4 | 4 | 7 | 4 | 3 | 3703.817(10) | 3709.817 | −6 |
| 7 | 4 | 3 | 7 | 4 | 4 | 3703.879(10) | 3711.879 | −8 |
| 6 | 4 | 2 | 6 | 4 | 3 | 3704.358(50) | 3738.358 | −34 |
| 6 | 4 | 3 | 6 | 4 | 2 | 3704.358(50) | 3720.358 | −16 |
| 5 | 4 | 1 | 5 | 4 | 2 | 3704.817(10) | 3731.817 | −27 |
| 5 | 4 | 2 | 5 | 4 | 1 | 3704.817(10) | 3727.817 | −23 |
| 6 | 2 | 4 | 5 | 3 | 3 | 3704.817(50) | 3733.817 | −29 |

      

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| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 3 | 1 | 2 | 2 | 2 | 1 | 3704.857(50) | 3722.857 | −18 |
| 0 | 0 | 0 | 1 | 0 | 1 | 3704.939(50) | 3684.939 | 20 |
| 4 | 4 | 0 | 4 | 4 | 1 | 3705.197(10) | 3676.197 | 29 |
| 4 | 4 | 1 | 4 | 4 | 0 | 3705.197(10) | 3734.197 | −29 |
| 6 | 2 | 5 | 6 | 2 | 4 | 3705.219(10) | 3417.219 | 288[*] |
| 8 | 3 | 6 | 8 | 3 | 5 | 3705.518(10) | 3714.518 | −9 |
| 3 | 1 | 3 | 3 | 1 | 2 | 3705.744(50) | 3724.744 | −19 |
| 7 | 3 | 5 | 7 | 3 | 4 | 3707.199(10) | 3713.199 | −6 |
| 5 | 1 | 5 | 4 | 2 | 2 | 3708.150(50) | 3705.150 | 3 |
| 6 | 3 | 4 | 6 | 3 | 3 | 3708.254(10) | 3723.254 | −15 |
| 1 | 1 | 1 | 2 | 0 | 2 | 3708.554(10) | 3724.554 | −16 |
| 5 | 2 | 4 | 5 | 2 | 3 | 3708.930(50) | 3584.930 | 124[*] |
| 5 | 3 | 3 | 5 | 3 | 2 | 3708.930(50) | 3720.930 | −12 |
| 6 | 3 | 3 | 6 | 3 | 4 | 3709.119(10) | 3744.119 | −35 |
| 4 | 3 | 2 | 4 | 3 | 1 | 3709.373(10) | 3716.373 | −7 |
| 4 | 3 | 1 | 4 | 3 | 2 | 3709.430(50) | 3734.430 | −25 |
| 3 | 3 | 1 | 3 | 3 | 0 | 3709.685(50) | 3700.685 | 9 |
| 3 | 3 | 0 | 3 | 3 | 1 | 3709.695(50) | 3701.695 | 8 |
| 8 | 3 | 5 | 8 | 3 | 6 | 3710.114(10) | 3737.114 | −27 |
| 2 | 1 | 2 | 2 | 1 | 1 | 3710.775(10) | 3722.775 | −12 |
| 4 | 2 | 3 | 4 | 2 | 2 | 3711.338(10) | 3638.338 | 73[*] |
| 6 | 1 | 6 | 5 | 2 | 3 | 3711.866(50) | 3672.866 | 39 |
| 3 | 2 | 2 | 3 | 2 | 1 | 3712.651(10) | 3699.257 | 13 |
| 2 | 2 | 1 | 2 | 2 | 0 | 3713.257(50) | 3742.257 | −29 |
| 2 | 2 | 0 | 2 | 2 | 1 | 3713.496(10) | 3739.496 | −26 |
| 3 | 2 | 1 | 3 | 2 | 2 | 3713.832(50) | 3694.832 | 19 |
| 1 | 1 | 1 | 1 | 1 | 0 | 3714.137(10) | 3714.137 | 0 |
| 4 | 2 | 2 | 4 | 2 | 3 | 3714.756(10) | 3685.756 | 29 |
| 5 | 2 | 3 | 5 | 2 | 4 | 3716.657(10) | 3692.657 | 24 |
| 5 | 2 | 3 | 5 | 2 | 4 | 3716.657(10) | 3692.657 | 24 |
| 1 | 1 | 0 | 1 | 1 | 1 | 3717.367(10) | 3709.367 | 8 |
| 4 | 1 | 3 | 3 | 2 | 2 | 3719.221(10) | 3728.221 | −9 |
| 4 | 2 | 2 | 5 | 1 | 5 | 3719.327(10) | 3692.327 | 27 |
| 6 | 2 | 4 | 6 | 2 | 5 | 3719.865(10) | 3700.865 | 19 |
| 2 | 1 | 1 | 2 | 1 | 2 | 3720.452(50) | 3713.452 | 7 |
| 2 | 0 | 2 | 1 | 1 | 1 | 3723.518(10) | 3698.518 | 25 |
| 2 | 2 | 1 | 3 | 1 | 2 | 3724.079(10) | 3725.079 | −1 |
| 7 | 2 | 5 | 7 | 2 | 6 | 3724.568(10) | 3716.568 | 8 |
| 3 | 1 | 2 | 3 | 1 | 3 | 3725.042(10) | 3735.042 | −10 |
| 1 | 0 | 1 | 0 | 0 | 0 | 3728.149(10) | 3712.149 | 36 |
| 8 | 2 | 6 | 8 | 2 | 7 | 3730.842(10) | 3718.842 | 12 |
| 4 | 1 | 3 | 4 | 1 | 4 | 3731.131(10) | 3740.131 | −9 |
| 4 | 3 | 2 | 5 | 2 | 3 | 3721.577(10) | 3693.577 | 28 |
| 1 | 1 | 0 | 1 | 0 | 1 | 3733.357(10) | 3725.357 | 8 |
| 5 | 1 | 4 | 4 | 2 | 3 | 3734.056(10) | 3735.056 | −1 |
| 2 | 1 | 1 | 2 | 0 | 2 | 3734.942(50) | 3748.942 | −14 |
| 4 | 3 | 1 | 5 | 2 | 4 | 3735.299(50) | 3723.299 | 12 |
| 3 | 0 | 3 | 2 | 1 | 2 | 3736.028(10) | 3719.028 | 17 |
| 2 | 1 | 2 | 1 | 1 | 1 | 3737.204(10) | 3737.204 | 0 |
| 3 | 1 | 2 | 3 | 0 | 3 | 3737.549(10) | 3744.549 | −7 |
| 5 | 1 | 4 | 5 | 1 | 5 | 3738.615(10) | 3753.615 | −15 |
| 2 | 0 | 2 | 1 | 0 | 1 | 3739.500(10) | 3723.500 | 16 |
| 2 | 1 | 1 | 1 | 1 | 0 | 3740.513(10) | 3750.513 | −10 |
| 4 | 1 | 3 | 4 | 0 | 4 | 3741.318(50) | 3770.318 | −29 |
| 1 | 1 | 1 | 0 | 0 | 0 | 3743.338(10) | 3747.338 | −4 |
| 5 | 1 | 4 | 5 | 0 | 5 | 3746.505(10) | 3762.505 | −16 |
| 6 | 1 | 5 | 6 | 1 | 6 | 3747.373(10) | 3765.373 | −18 |
| 3 | 1 | 3 | 2 | 1 | 2 | 3747.668(10) | 3759.668 | −12 |
| 3 | 2 | 2 | 2 | 2 | 1 | 3748.046(10) | 3725.046 | 23 |
| 3 | 2 | 1 | 2 | 2 | 0 | 3748.544(10) | 3738.544 | 10 |
| 4 | 0 | 4 | 3 | 1 | 3 | 3748.608(10) | 3739.608 | 9 |
| 6 | 1 | 5 | 5 | 2 | 4 | 3749.199(10) | 3755.199 | −6 |
| 3 | 0 | 3 | 2 | 0 | 2 | 3750.541(10) | 3732.541 | 18 |
| 3 | 1 | 2 | 2 | 1 | 1 | 3752.710(10) | 3764.710 | −12 |
| 2 | 1 | 2 | 1 | 0 | 1 | 3753.185(10) | 3763.185 | −10 |
| 6 | 1 | 5 | 6 | 0 | 6 | 3753.185(50) | 3753.185 | 0 |
| 6 | 2 | 4 | 6 | 1 | 5 | 3754.397(10) | 3742.397 | 12 |
| 7 | 2 | 5 | 7 | 1 | 6 | 3754.468(10) | 3754.468 | 0 |
| 5 | 2 | 3 | 5 | 1 | 4 | 3755.434(10) | 3730.434 | 25 |

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| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 8 | 2 | 6 | 8 | 1 | 7 | 3755.919(10) | 3746.919 | 9 |
| 4 | 3 | 2 | 3 | 3 | 1 | 3755.994(50) | 3740.994 | 15 |
| 4 | 3 | 1 | 3 | 3 | 0 | 3756.024(50) | 3746.024 | 8 |
| 4 | 2 | 2 | 4 | 1 | 3 | 3757.218(10) | 3735.218 | 22 |
| 4 | 1 | 4 | 3 | 1 | 3 | 3757.948(10) | 3773.948 | −16 |
| 9 | 2 | 9 | 7 | 1 | 8 | 3758.901(10) | 3850.901 | 8 |
| 3 | 2 | 1 | 3 | 1 | 2 | 3759.322(50) | 3764.322 | −5 |
| 4 | 2 | 3 | 3 | 2 | 2 | 3759.322(50) | 3676.322 | 83* |
| 4 | 2 | 2 | 3 | 2 | 1 | 3760.535(10) | 3743.535 | 17 |
| 5 | 0 | 5 | 4 | 1 | 4 | 3760.953(10) | 3748.953 | 12 |
| 4 | 0 | 4 | 3 | 0 | 3 | 3761.107(10) | 3757.107 | 4 |
| 7 | 1 | 6 | 7 | 0 | 7 | 3761.276(10) | 3770.276 | −9 |
| 2 | 2 | 0 | 2 | 1 | 1 | 3761.348(10) | 3783.348 | −22 |
| 3 | 1 | 3 | 2 | 0 | 2 | 3762.176(10) | 3778.176 | −16 |
| 5 | 4 | 1 | 4 | 4 | 0 | 3762.870(10) | 3780.870 | −18 |
| 5 | 4 | 2 | 4 | 4 | 1 | 3762.870(10) | 3776.870 | −16 |
| 10 | 2 | 8 | 10 | 1 | 9 | 3763.546(10) | 3749.546 | 14 |
| 7 | 1 | 6 | 6 | 2 | 5 | 3764.473(10) | 3763.473 | 1 |
| 4 | 1 | 3 | 3 | 1 | 2 | 3764.730(10) | 3779.730 | −15 |
| 2 | 2 | 1 | 2 | 1 | 2 | 3765.979(10) | 3783.979 | −18 |
| 5 | 3 | 3 | 4 | 3 | 2 | 3767.325(10) | 3773.325 | −6 |
| 5 | 3 | 2 | 4 | 3 | 1 | 3765.453(10) | 3774.453 | −9 |
| 5 | 1 | 5 | 4 | 1 | 4 | 3768.021(10) | 3777.021 | −9 |
| 3 | 2 | 2 | 3 | 1 | 3 | 3768.228(10) | 3740.228 | 28 |
| 6 | 5 | 2 | 5 | 5 | 1 | 3769.881(10) | 3805.881 | −36 |
| 6 | 5 | 1 | 5 | 5 | 0 | 3769.881(10) | 3805.881 | −36 |
| 11 | 3 | 8 | 11 | 2 | 9 | 3770.189(10) | 3762.189 | 8 |
| 4 | 1 | 4 | 3 | 0 | 3 | 3770.439(50) | 3799.439 | −29 |
| 5 | 2 | 4 | 4 | 2 | 3 | 3770.439(50) | 3601.439 | 169* |
| 8 | 1 | 7 | 8 | 0 | 8 | 3770.593(10) | 3768.593 | 2 |
| 5 | 0 | 5 | 4 | 0 | 4 | 3771.163(10) | 3756.163 | 15 |
| 4 | 2 | 3 | 4 | 1 | 4 | 3771.245(10) | 3675.245 | 96* |
| 10 | 3 | 7 | 10 | 2 | 8 | 3772.669(10) | 3781.669 | −9 |
| 5 | 2 | 3 | 4 | 2 | 2 | 3772.777(10) | 3779.777 | 7 |
| 6 | 0 | 6 | 5 | 1 | 5 | 3772.819(10) | 3734.819 | 38 |
| 6 | 4 | 2 | 5 | 4 | 1 | 3774.061(10) | 3800.061 | −26 |
| 6 | 4 | 3 | 5 | 4 | 2 | 3774.061(10) | 3791.061 | −17 |
| 5 | 2 | 4 | 5 | 1 | 5 | 3775.010(10) | 3608.010 | 167* |
| 9 | 3 | 6 | 9 | 2 | 7 | 3776.061(10) | 3793.061 | −17 |
| 5 | 1 | 4 | 4 | 1 | 3 | 3776.516(10) | 3786.516 | −10 |
| 12 | 2 | 10 | 12 | 1 | 11 | 3777.718(10) | 3765.718 | 12 |
| 6 | 1 | 6 | 5 | 1 | 5 | 3777.858(10) | 3781.858 | −4 |
| 5 | 1 | 5 | 4 | 0 | 4 | 3778.226(10) | 3789.226 | −11 |
| 6 | 3 | 4 | 5 | 3 | 3 | 3778.610(10) | 3789.610 | −11 |
| 6 | 3 | 3 | 5 | 3 | 2 | 3778.950(10) | 3801.950 | −23 |
| 6 | 2 | 5 | 6 | 1 | 6 | 3779.601(10) | 3450.601 | 329* |
| 8 | 3 | 5 | 8 | 2 | 6 | 3779.904(10) | 3794.904 | −15 |
| 6 | 0 | 6 | 5 | 0 | 5 | 3780.716(10) | 3735.716 | 45 |
| 7 | 5 | 3 | 6 | 5 | 2 | 3780.874(10) | 3778.874 | 2 |
| 7 | 5 | 2 | 6 | 5 | 1 | 3780.874(10) | 3778.874 | 2 |
| 6 | 2 | 5 | 5 | 2 | 4 | 3781.421(10) | 3446.421 | 335* |
| 7 | 3 | 4 | 7 | 2 | 5 | 3783.693(10) | 3802.693 | −19 |
| 7 | 0 | 7 | 6 | 1 | 6 | 3784.088(10) | 3677.088 | 107* |
| 6 | 2 | 4 | 5 | 2 | 3 | 3785.251(10) | 3770.251 | 15 |
| 6 | 1 | 6 | 5 | 0 | 5 | 3785.755(10) | 3784.755 | 1 |
| 2 | 2 | 1 | 1 | 1 | 0 | 3786.069(10) | 3793.069 | −7 |
| 6 | 3 | 3 | 6 | 2 | 4 | 3787.024(10) | 3800.024 | −13 |
| 7 | 1 | 7 | 6 | 1 | 6 | 3787.478(10) | 3767.478 | 20 |
| 2 | 2 | 0 | 1 | 1 | 1 | 3787.775(10) | 3809.775 | −22 |
| 6 | 1 | 5 | 5 | 1 | 4 | 3787.963(10) | 3805.963 | −18 |
| 5 | 3 | 2 | 5 | 2 | 3 | 3789.632(10) | 3789.632 | 0 |
| 7 | 0 | 7 | 6 | 0 | 6 | 3789.883(10) | 3680.883 | 109* |
| 7 | 3 | 4 | 6 | 3 | 3 | 3790.601(10) | 3802.601 | −12 |
| 4 | 3 | 1 | 4 | 2 | 2 | 3791.438(10) | 3777.601 | 14 |
| 4 | 3 | 2 | 4 | 2 | 3 | 3793.025(10) | 3781.025 | 12 |
| 3 | 3 | 1 | 3 | 2 | 2 | 3793.088(10) | 3763.088 | 30 |
| 5 | 3 | 3 | 5 | 2 | 4 | 3793.165(10) | 3791.165 | 2 |
| 7 | 1 | 7 | 6 | 0 | 6 | 3793.274(10) | 3770.274 | 23 |
| 6 | 3 | 4 | 6 | 2 | 5 | 3793.617(10) | 3796.617 | −3 |
| 8 | 0 | 8 | 7 | 1 | 7 | 3794.388(10) | 3653.388 | 141* |
| 7 | 3 | 5 | 7 | 2 | 6 | 3794.499(10) | 3793.499 | 1 |

    

where $E_v^i$ is the vibrationnal energy of the $i$ state and $E_r\left(J, K_a, K_c : P^i\right)$ represents the rotational energy of the $J$, $K_a$, $K_c$ level, calculated with the efficient Hamiltonian given by the Equation (14) for the $P^i$ spectroscopic parameter of the $i$ vibrationnal state.

In this work, the $P^0$ spectroscopic parameters of the fundamental state have been considered equal to the Helminger's values published in [21] and $E_v^0$ arbitrarily fixed at zero. The $P^1$ spectroscopic parameters of the vibrationnal state $v_1 = 1$ has been determined by adjustment using the least squares program. The results of the analysis are in the **Tables 2** and **3**.

## 2.2. The $v_1(v_3)$ Band Intensity

To calculate the transitions intensity, it is necessary for us to determine, at first, the dipolar momentum function.

### 2.2.1. Determination of the Dipolar Momentum Function

From the $S_1$ and $S_2$ coordinates corresponding respectively to the following small variations $\Delta r_{31}$ and $\Delta r_{32}$ of the inter atomic distances and $S_3$ corresponding to small variations of the valence angle $\Delta\Phi$, the Schrödinger equation for the vibration [22] becomes:

$$H_v = \frac{1}{2}\sum_{i,j=1}^{3} G_{ij} P_i P_j + \frac{1}{2}\sum_{i,j=1}^{3} F_{ij} S_i S_j \qquad (16)$$

where $P_i = \dfrac{-i\partial}{\partial S_i}$ is the conjugated momentum of the co-ordinate $S_i$, $G$ and $F$ correspond respectively to the kinetic and potential energies and can be calculated numerically from the Wilson Equation [22] once the molecule's equilibrium configuration is known. The $F$ tensor components can be calculated numerically using Patridge and Schwenke [6] potential energy surface. The $H_v$ eigenenergies were obtained by solving the following equation:

$$FX = \lambda G^{-1} X \qquad (17)$$

where $\lambda$ and $X$ are respectively eigenvalue and eigenvector.

Thus we can deduce the equation permitting the passage from normal dimensionless coordinates $q_k$ to the internal coordinates.

$$S_i = \sum_{k=1}^{3}\left(\frac{X_i^k}{\lambda_k^{1/4}}\right) q_k \qquad (18)$$

Then we try to obtain the dipolar momentum function according to the internal coordinates:

$$\mu_x = {}^s\mu_x^0 + \sum_{i=1}^{3} {}^s\mu_x^i S_i$$

and

$$\mu_z = {}^s\mu_z^0 + \sum_{i=1}^{3} {}^s\mu_z^i S_i \qquad (19)$$

**Table 3. The spectroscopic constants of the fundamental and the $v_1(v_3)$ band of HTO.**

| | Constant value to the $v_1(v_3)$ band | | Constant value to the fundamental |
|---|---|---|---|
| $E^1$ | 3716.5475(48) | $E^0$ | 0 |
| $A$ | 21.8482(37) | $A$ | 22.61061 |
| $B$ | 6.58908(75) | $B$ | 6.61116 |
| $C$ | 4.97656(72) | $C$ | 5.01889 |
| $\Delta_K$ | $13.796(810) \times 10^{-3}$ | $\Delta_K$ | $9.04872 \times 10^{-3}$ |
| $\Delta_{KJ}$ | $2.306(130) \times 10^{-3}$ | $\Delta_{KJ}$ | $1.61856 \times 10^{-3}$ |
| $\Delta_J$ | $0.1628(71) \times 10^{-3}$ | $\Delta_J$ | $0.17385 \times 10^{-3}$ |
| $\delta_K$ | $-6.710(320) \times 10^{-3}$ | $\delta_K$ | $1.71208 \times 10^{-3}$ |
| $\delta J$ | $16.670(390) \times 10^{-6}$ | $\delta J$ | $47.1697 \times 10^{-6}$ |
| $H_K$ | $888.900(680) \times 10^{-6}$ | $H_K$ | $29.880 \times 10^{-6}$ |
| $H_{KJ}$ | $127.500(160) \times 10^{-6}$ | $H_{KJ}$ | $-2.110 \times 10^{-6}$ |
| $H_{JK}$ | $-24.000(18) \times 10^{-6}$ | $H_{JK}$ | $1.316 \times 10^{-6}$ |
| $H_J$ | $-0.224(64) \times 10^{-6}$ | $H_J$ | $17.337 \times 10^{-9}$ |
| $h_K$ | $-894.900(360 \times 10^{-6}$ | $h_K$ | $17.947 \times 10^{-6}$ |
| $h_{KJ}$ | $-35.500(270) \times 10^{-6}$ | $h_{KJ}$ | $0.5713 \times 10^{-6}$ |
| $h_J$ | $-0.140(16) \times 10^{-6}$ | $h_J$ | $5.946 \times 10^{-9}$ |
| $L_K$ | $-20.000(24) \times 10^{-6}$ | $L_K$ | $-0.277 \times 10^{-6}$ |
| $L_{KKJ}$ | $-11.130(50) \times 10^{-6}$ | $L_{KKJ}$ | $0.0659 \times 10^{-6}$ |
| $L_{KJ}$ | $1.906(120) \times 10^{-6}$ | $L_{KJ}$ | $-0.018 \times 10^{-6}$ |
| $L_{KJJ}$ | $0.0831(90) \times 10^{-6}$ | | |
| $L_J$ | $0.404(180) \times 10^{-9}$ | $l_K$ | $-0.2713 \times 10^{-6}$ |
| $I_K$ | $29.781(1600) \times 10^{-6}$ | $l_{KJ}$ | $-3.0395 \times 10^{-9}$ |
| $I_{KJ}$ | $0.924(80) \times 10^{-6}$ | | |
| $I_{JK}$ | $89.840(760) \times 10^{-9}$ | $P_K$ | $3.673 \times 10^{-9}$ |
| $P_K$ | $238.400(300) \times 10^{-9}$ | | |
| $P_{KKKJ}$ | $115.200(100) \times 10^{-9}$ | $p_K$ | $0.969 \times 10^{-9}$ |
| $p_K$ | $-196.900(150) \times 10^{-9}$ | | |

where $^{s}\mu_{\alpha}^{0}$ with $\alpha = x$ or $z$ and $^{s}\mu_{\alpha}^{i}$ with $1 \le i \le 3$ are constants.

To determine the HTO dipolar momentum function, we use the unvariability of this function with an isotopic substitution when it is expressed by the internal coordinates. However, it will be necessary to take to account the way from which the molecule depending reference mark *O'xyz* is going to change.

From the Equation (18) and by replacing the $S_i$ by the $q_i$ in the Equation (19), we find the HTO dipolar momentum function expressed in the normal dimensionless coordinates. Considering the Equation (18), the terms $X_i^k$ and $\lambda_k$ will have the values corresponding to the HTO normal modes and the results are shown in the **Table 4**.

### 2.2.2. The Absorption Band Intensity

The intensity of a molecular absorption band, in a gas at the thermodynamic equilibrium [23], is given as followed:

$$S_A^B = \frac{8\pi^3 g_A \sigma_{AB}}{3hcQ} 10^{-36} \exp\left(-\frac{hcE_A}{KT}\right)$$
$$\cdot\left[1 - \exp\left(-\frac{hc\sigma_{AB}}{KT}\right)\right]\left|\langle A|\mu_Z'|B\rangle\right|^2 \quad (20)$$

where $S_A^B$ is the intensity in cm$^{-1}$/(molécule·cm$^{-2}$) for a transition from the lower level A to the up level B at the $T$ temperature; $g_A$ is the degenerancy due to the nuclear spin of the lower level A; $\sigma_{AB}$ is the transition wave number in cm$^{-1}$;

$E_A$ is the lower energy level in cm$^{-1}$; $Q$ the distribution's function; $K$ the Boltzmann's constant and $\mu_Z'$ is the modified transition momentum in Debye. Its expression [23] is:

$$\mu_Z' = \Phi_x \mu_x + \Phi_z \mu_z \quad (21)$$

where $\mu_x$ and $\mu_z$ are the dipolar momentum components, in the reference mark related to the molecule, expressed according to the normal dimensionless coordinates. $\Phi_x$ and $\Phi_z$ are operators [23] depending to the vibrational coordinates which matrix elements are given in the **Tables 5** and **6**.

From the **Tables 3** and **5**, the wave number and the

**Table 4. Thevalues of the coefficients used in the development of the dipolar momentum function.**

| Coefficients | Valeur | Coefficients | Valeur |
|---|---|---|---|
| $\mu_x^0$ | −1.74117 | $\mu_z^0$ | −0.84923 |
| $\mu_x^1 \times 2^{1/2}$ | −0.01060 | $\mu_z^1 \times 2^{1/2}$ | −0.03502 |
| $\mu_x^2 \times 2^{1/2}$ | 0.10583 | $\mu_z^2 \times 2^{1/2}$ | −0.05269 |
| $\mu_x^3 \times 2^{1/2}$ | −0.03039 | $\mu_z^3 \times 2^{1/2}$ | 0.04091 |

intensity of the authorized transitions have been calculated using Equations (15) and (20), for $J \le 11$, for a temperature of 296 K.

The **Table 7** gives the portion of list covering the region 3630 to 3760 cm$^{-1}$ for the transitions which intensity is over $10^{-23}$ cm$^{-1}/($molecule·cm$^{-2})$.

## 3. Results and Discussion

### 3.1. Analysis of Waves Numbers

In this analysis, the efficient hamiltonian spectroscopic parameters of the Equation (14) and the vibrational energy have been considered.

The mean quadratic gap $q = 0.018$ cm$^{-1}$ is enough close to the experimental one for the observed wave number: 0.010 cm$^{-1}$. It is also possible to evaluate the quality of the analysis with the standard deviation $\sigma = 1.7$. Ideally, this value should be very close to 1. This excess can be the consequence of the underestimation of the experimental uncertainties and the use of an unadequate efficient Hamiltonian. In this latter, it can come from a perturbation of the superior vibrationnal state. This hypothesis is confirmed by the results in the **Table 2** for the transitions presenting a big gap (Obs.-Cal.) or even those that have been excluded in the analysis (in asterisk in the **Table 2**).

One realizes that these transitions often share the same superior rotationnal level and that the gap (Obs.-Cal.) is practically independent of the low level.

The **Table 8** illustrates well this fact for transitions excluded in the analysis for which the superior rotationnal levels are $8_{08}$ and $6_{25}$.

Presumably, the vibrationnal state $v_1 = 1$ is not isolated. It exists another closed vibrationnal state which is coupled whith it. To make a correct calculation of the vibrationnal energy, it would be necessary to treat simultaneously these two states. A calculation based on **Table 1**

**Table 5. The non zero elements matrix [23] operator $\Phi_z$.**

| $\Delta J$ | $\Delta K$ | $\Gamma$ | $\langle J, K, \gamma|\Phi_z| J', K', \gamma'\rangle$ |
|---|---|---|---|
| 0 | 0 | $-\gamma'$ | $K\left[(2J+1)/J(J+1)\right]^{1/2}$ |
| ±1 | 0 | $+\gamma'$ | $K\left[(m^2 - K^2)/|m|\right]^{1/2}$ |

**Table 6. The non zero elements matrix [23] operator $\Phi_x$.**

| $\Delta J$ | $\Delta K$ | $\Gamma$ | $\langle J, K, \gamma|\Phi_z| J', K', \gamma'\rangle$ |
|---|---|---|---|
| 0 | ±1 | $-\gamma'$ | $\frac{1}{2}\left\{\left[(2J+1)(J-K\Delta K)(J+1+K\Delta K)\right]/J(J+1)\right\}^{1/2}$ |
| ±1 | ±1 | $+\gamma'$ | $-\frac{1}{2}\Delta J\Delta K\left[(m+K\Delta K)(m+1+K\Delta K)/|m|\right]^{1/2}$ |

**Table 7. Waves numbers and lines intensities of $v_1(v_3)$ band of HTO.**

| $J'$ | $K'_a$ | $K'_c$ | $J''$ | $K''_a$ | $K''_c$ | Cal | S |
|---|---|---|---|---|---|---|---|
| 2 | 1 | 1 | 3 | 1 | 2 | 3678.528 | 6.47e−20 |
| 2 | 2 | 1 | 3 | 2 | 2 | 3678.564 | 3.24e−20 |
| 1 | 0 | 1 | 2 | 1 | 2 | 3678.828 | 2.22e−19 |
| 7 | 1 | 6 | 6 | 3 | 3 | 3679.121 | 1.00e−22 |
| 2 | 1 | 2 | 3 | 1 | 3 | 3683.118 | 6.79e−20 |
| 9 | 2 | 8 | 9 | 2 | 7 | 3683.043 | 1.34e−21 |
| 3 | 0 | 3 | 2 | 2 | 0 | 3683.299 | 7.21e−23 |
| 5 | 0 | 5 | 5 | 1 | 4 | 3683.695 | 2.59e−19 |
| 11 | 4 | 8 | 10 | 5 | 5 | 3684.293 | 1.31e−21 |
| 7 | 3 | 5 | 8 | 2 | 6 | 3684.665 | 1.67e−20 |
| 10 | 3 | 7 | 11 | 2 | 10 | 3685.350 | 2.63e−21 |
| 11 | 4 | 7 | 10 | 5 | 6 | 3685.575 | 1.31e−21 |
| 8 | 3 | 6 | 7 | 4 | 3 | 3685.976 | 6.99e−21 |
| 5 | 2 | 4 | 4 | 3 | 1 | 3686.796 | 1.60e−20 |
| 8 | 3 | 5 | 7 | 4 | 4 | 3688.519 | 7.03e−21 |
| 0 | 0 | 0 | 1 | 1 | 1 | 3688.927 | 1.65e−19 |
| 10 | 4 | 6 | 11 | 3 | 9 | 3689.439 | 2.45e−21 |
| 9 | 3 | 6 | 10 | 2 | 9 | 3689.711 | 5.18e−21 |
| 4 | 0 | 4 | 4 | 1 | 3 | 3689.714 | 3.32e−19 |
| 5 | 1 | 5 | 5 | 1 | 4 | 3690.785 | 5.34e−21 |
| 5 | 2 | 3 | 4 | 3 | 2 | 3690.802 | 1.65e−20 |
| 1 | 1 | 0 | 2 | 1 | 1 | 3690.941 | 4.38e−20 |
| 11 | 0 | 11 | 10 | 2 | 8 | 3692.047 | 3.26e−21 |
| 8 | 2 | 7 | 8 | 2 | 6 | 3691.788 | 2.66e−21 |
| 8 | 1 | 7 | 7 | 3 | 4 | 3692.310 | 1.28e−22 |
| 11 | 1 | 11 | 10 | 2 | 8 | 3692.615 | 9.26e−22 |
| 4 | 0 | 4 | 3 | 2 | 1 | 3693.035 | 2.21e−22 |
| 1 | 0 | 1 | 2 | 0 | 2 | 3693.340 | 6.41e−20 |
| 9 | 4 | 6 | 10 | 3 | 7 | 3693.679 | 4.01e−21 |
| 11 | 3 | 9 | 11 | 3 | 8 | 3693.883 | 5.50e−22 |
| 4 | 2 | 3 | 5 | 1 | 4 | 3693.985 | 5.86e−20 |
| 1 | 1 | 1 | 2 | 1 | 2 | 3694.058 | 4.49e−20 |
| 3 | 0 | 3 | 3 | 1 | 2 | 3694.093 | 3.70e−19 |
| 3 | 1 | 3 | 2 | 2 | 0 | 3694.968 | 1.73e−20 |
| 2 | 1 | 2 | 3 | 0 | 3 | 3695.622 | 1.67e−19 |
| 8 | 3 | 5 | 9 | 2 | 5 | 3696.172 | 8.99e−21 |
| 8 | 8 | 1 | 9 | 8 | 2 | 3696.388 | 3.63e−23 |
| 8 | 8 | 0 | 9 | 8 | 1 | 3696.388 | 3.63e−23 |
| 11 | 5 | 7 | 11 | 5 | 6 | 3696.552 | 5.29e−22 |
| 11 | 5 | 6 | 11 | 5 | 7 | 3696.653 | 5.29e−22 |
| 6 | 2 | 5 | 5 | 3 | 2 | 3697.186 | 1.96e−20 |
| 2 | 0 | 2 | 2 | 1 | 1 | 3697.075 | 3.45e−19 |
| 9 | 3 | 7 | 8 | 4 | 4 | 3697.116 | 5.87e−21 |
| 11 | 6 | 6 | 11 | 6 | 5 | 3697.356 | 3.24e−22 |
| 11 | 6 | 5 | 11 | 6 | 6 | 3697.359 | 3.24e−22 |
| 10 | 5 | 6 | 10 | 5 | 5 | 3697.498 | 1.08e−21 |
| 10 | 5 | 5 | 10 | 5 | 6 | 3697.537 | 1.08e−21 |
| 10 | 6 | 5 | 10 | 6 | 4 | 3697.724 | 6.62e−22 |
| 10 | 6 | 4 | 10 | 6 | 5 | 3697.725 | 6.62e−22 |
| 9 | 6 | 4 | 9 | 6 | 3 | 3698.201 | 1.29e−21 |
| 9 | 6 | 3 | 9 | 6 | 4 | 3698.201 | 1.29e−21 |
| 9 | 8 | 2 | 10 | 8 | 3 | 3698.205 | 3.99e−23 |
| 9 | 8 | 1 | 10 | 8 | 2 | 3698.205 | 3.99e−23 |
| 9 | 5 | 5 | 9 | 5 | 4 | 3698.358 | 2.11e−21 |
| 9 | 5 | 4 | 9 | 5 | 5 | 3698.371 | 2.11e−21 |
| 9 | 9 | 0 | 10 | 10 | 1 | 3698.568 | 2.66e−23 |
| 9 | 9 | 1 | 10 | 10 | 0 | 3698.568 | 2.66e−23 |
| 8 | 6 | 3 | 8 | 6 | 2 | 3698.679 | 2.39e−21 |
| 8 | 6 | 2 | 8 | 6 | 3 | 3698.679 | 2.39e−21 |
| 1 | 0 | 1 | 1 | 1 | 0 | 3698.907 | 2.46e−19 |
| 4 | 1 | 4 | 4 | 1 | 3 | 3699.079 | 8.72e−21 |
| 7 | 6 | 2 | 7 | 6 | 1 | 3699.123 | 4.26e−21 |
| 7 | 6 | 1 | 7 | 6 | 2 | 3699.123 | 4.26e−21 |

**Continued**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 8 | 5 | 4 | 8 | 5 | 3 | 3699.147 | 3.94e−21 |
| 7 | 5 | 3 | 7 | 5 | 2 | 3699.863 | 7.03e−21 |
| 7 | 5 | 2 | 7 | 5 | 3 | 3699.864 | 7.03e−21 |
| 11 | 4 | 8 | 11 | 4 | 7 | 3700.237 | 6.63e−22 |
| 6 | 5 | 2 | 6 | 5 | 1 | 3700.500 | 1.21e−21 |
| 6 | 5 | 1 | 6 | 5 | 2 | 3700.500 | 1.21e−20 |
| 10 | 0 | 10 | 9 | 2 | 7 | 3700.500 | 7.10e−21 |
| 5 | 5 | 1 | 5 | 5 | 0 | 3701.048 | 2.00e−20 |
| 5 | 5 | 0 | 5 | 5 | 1 | 3701.048 | 2.00e−20 |
| 5 | 0 | 5 | 4 | 2 | 2 | 3701.056 | 3.72e−22 |
| 9 | 4 | 5 | 10 | 3 | 8 | 3701.063 | 3.95e−21 |
| 6 | 3 | 4 | 7 | 2 | 5 | 3701.368 | 2.00e−20 |
| 10 | 1 | 10 | 9 | 2 | 7 | 3701.418 | 2.13e−21 |
| 10 | 4 | 7 | 10 | 4 | 6 | 3701.470 | 1.38e−21 |
| 9 | 3 | 6 | 8 | 4 | 5 | 3701.986 | 5.92e−21 |
| 4 | 1 | 4 | 3 | 2 | 1 | 3702.401 | 2.87e−20 |
| 9 | 4 | 6 | 9 | 4 | 5 | 3702.414 | 2.72e−21 |
| 11 | 4 | 7 | 11 | 4 | 8 | 3702.529 | 6.65e−22 |
| 10 | 4 | 6 | 10 | 4 | 7 | 3702.573 | 1.38e−21 |
| 9 | 4 | 5 | 9 | 4 | 6 | 3702.899 | 2.72e−21 |
| 9 | 3 | 7 | 9 | 3 | 6 | 3702.953 | 2.47e−21 |
| 8 | 4 | 5 | 8 | 4 | 4 | 3703.180 | 5.10e−21 |
| 8 | 4 | 4 | 8 | 4 | 5 | 3703.370 | 5.10e−21 |
| 7 | 4 | 4 | 7 | 4 | 3 | 3703.825 | 9.14e−21 |
| 7 | 4 | 3 | 7 | 4 | 4 | 3703.889 | 9.14e−21 |
| 9 | 1 | 8 | 8 | 3 | 5 | 3703.941 | 1.34e−22 |
| 7 | 3 | 4 | 8 | 2 | 7 | 3704.346 | 1.36e−20 |
| 6 | 4 | 3 | 6 | 4 | 2 | 3704.376 | 1.57e−20 |
| 6 | 4 | 2 | 6 | 4 | 3 | 3704.393 | 1.57e−20 |
| 5 | 4 | 2 | 5 | 4 | 1 | 3704.842 | 2.62e−20 |
| 5 | 4 | 1 | 5 | 4 | 2 | 3704.845 | 2.62e−20 |
| 6 | 2 | 4 | 5 | 3 | 3 | 3704.847 | 2.09e−20 |
| 3 | 1 | 2 | 2 | 2 | 1 | 3704.876 | 2.33e−20 |
| 0 | 0 | 0 | 1 | 0 | 1 | 3704.918 | 3.60e−20 |
| 6 | 2 | 5 | 6 | 2 | 4 | 3705.251 | 9.30e−21 |
| 4 | 4 | 1 | 4 | 4 | 0 | 3705.227 | 4.28e−20 |
| 4 | 4 | 0 | 4 | 4 | 1 | 3705.227 | 4.28e−20 |
| 8 | 3 | 6 | 8 | 3 | 5 | 3705.528 | 4.79e−21 |
| 9 | 3 | 6 | 10 | 1 | 9 | 3705.534 | 1.63e−23 |
| 3 | 1 | 3 | 3 | 1 | 2 | 3705.763 | 1.43e−20 |
| 7 | 2 | 6 | 6 | 3 | 3 | 3706.308 | 1.90e−20 |
| 9 | 0 | 9 | 8 | 2 | 6 | 3706.420 | 1.41e−22 |
| 6 | 0 | 6 | 5 | 2 | 3 | 3706.744 | 4.28e−22 |
| 10 | 8 | 3 | 11 | 8 | 4 | 3706.895 | 3.13e−23 |
| 10 | 8 | 2 | 11 | 8 | 3 | 3706.895 | 3.13e−23 |
| 7 | 3 | 5 | 7 | 3 | 4 | 3707.206 | 8.77e−21 |
| 9 | 1 | 9 | 8 | 2 | 6 | 3707.885 | 4.60e−21 |
| 10 | 3 | 8 | 9 | 4 | 5 | 3707.903 | 4.37e−21 |
| 5 | 1 | 5 | 4 | 2 | 2 | 3708.146 | 3.01e−20 |
| 6 | 3 | 4 | 6 | 3 | 3 | 3708.269 | 1.53e−20 |
| 1 | 1 | 1 | 2 | 0 | 2 | 3708.570 | 9.17e−20 |
| 5 | 2 | 4 | 5 | 2 | 3 | 3708.964 | 1.62e−20 |
| 5 | 3 | 3 | 5 | 3 | 2 | 3708.943 | 2.57e−20 |
| 8 | 4 | 5 | 9 | 3 | 6 | 3709.016 | 5.76e−21 |
| 6 | 3 | 3 | 6 | 3 | 5 | 3709.155 | 1.53e−20 |
| 5 | 3 | 2 | 5 | 3 | 3 | 3709.242 | 2.57e−20 |
| 3 | 2 | 2 | 4 | 1 | 3 | 3709.316 | 4.58e−20 |
| 7 | 3 | 4 | 7 | 3 | 5 | 3709.370 | 8.78e−21 |
| 4 | 3 | 2 | 4 | 3 | 1 | 3709.380 | 4.21e−20 |
| 4 | 3 | 1 | 4 | 3 | 2 | 3709.456 | 4.21e−20 |
| 8 | 0 | 8 | 7 | 2 | 5 | 3709.349 | 2.48e−22 |
| 7 | 0 | 7 | 6 | 2 | 4 | 3709.746 | 3.66e−22 |
| 3 | 3 | 1 | 3 | 3 | 0 | 3709.676 | 6.87e−20 |
| 3 | 3 | 0 | 3 | 3 | 1 | 3709.687 | 6.87e−20 |
| 3 | 3 | 0 | 3 | 3 | 1 | 3709.687 | 6.87e−20 |

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| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 8 | 3 | 5 | 8 | 3 | 6 | 3710.140 | 4.81e−21 |
| 2 | 1 | 2 | 2 | 1 | 1 | 3710.787 | 2.45e−20 |
| 4 | 2 | 3 | 4 | 2 | 2 | 3711.346 | 2.74e−20 |
| 9 | 3 | 6 | 9 | 3 | 7 | 3711.777 | 2.50e−21 |
| 8 | 1 | 8 | 7 | 2 | 5 | 3711.699 | 9.11e−21 |
| 6 | 1 | 6 | 5 | 2 | 3 | 3711.826 | 2.42e−20 |
| 6 | 2 | 4 | 7 | 1 | 7 | 3712.596 | 1.30e−20 |
| 3 | 2 | 2 | 3 | 2 | 1 | 3712.637 | 4.53e−20 |
| 7 | 2 | 5 | 8 | 1 | 8 | 3712.803 | 7.01e−21 |
| 7 | 1 | 7 | 6 | 2 | 4 | 3713.116 | 1.60e−20 |
| 8 | 4 | 4 | 9 | 3 | 7 | 3713.161 | 5.72e−21 |
| 2 | 2 | 1 | 2 | 2 | 0 | 3713.286 | 7.74e−20 |
| 7 | 7 | 1 | 7 | 7 | 0 | 3713.305 | 2.10e−21 |
| 7 | 7 | 0 | 7 | 7 | 1 | 3713.305 | 2.10e−21 |
| 10 | 1 | 9 | 9 | 3 | 6 | 3713.361 | 1.15e−22 |
| 10 | 5 | 6 | 11 | 4 | 7 | 3713.442 | 1.14e−21 |
| 2 | 2 | 0 | 2 | 2 | 1 | 3713.523 | 7.74e−20 |
| 3 | 2 | 1 | 3 | 2 | 2 | 3713.812 | 4.54e−20 |
| 6 | 3 | 3 | 7 | 2 | 6 | 3713.825 | 1.79e−20 |
| 1 | 1 | 1 | 1 | 1 | 0 | 3714.137 | 4.97e−20 |
| 10 | 5 | 5 | 11 | 4 | 8 | 3714.491 | 1.14e−21 |
| 10 | 3 | 7 | 10 | 3 | 8 | 3714.599 | 1.23e−21 |
| 8 | 2 | 7 | 7 | 3 | 4 | 3714.328 | 1.55e−20 |
| 4 | 2 | 2 | 4 | 2 | 3 | 3714.727 | 2.75e−20 |
| 5 | 2 | 3 | 6 | 1 | 6 | 3714.819 | 2.10e−20 |
| 8 | 7 | 2 | 8 | 7 | 1 | 3715.312 | 1.19e−21 |
| 8 | 7 | 1 | 8 | 7 | 2 | 3715.312 | 1.19e−21 |
| 8 | 2 | 6 | 9 | 1 | 9 | 3715.443 | 3.39e−21 |
| 7 | 2 | 5 | 8 | 0 | 8 | 3715.547 | 4.75e−23 |
| 10 | 3 | 7 | 9 | 4 | 6 | 3716.434 | 4.50e−21 |
| 8 | 3 | 5 | 9 | 1 | 8 | 3716.471 | 2.30e−23 |
| 5 | 2 | 3 | 5 | 2 | 4 | 3716.633 | 1.64e−20 |
| 6 | 2 | 4 | 7 | 0 | 7 | 3716.660 | 8.90e−23 |
| 5 | 3 | 3 | 6 | 2 | 4 | 3717.007 | 2.10e−20 |
| 8 | 2 | 6 | 9 | 0 | 9 | 3717.241 | 2.12e−23 |
| 1 | 1 | 0 | 1 | 1 | 1 | 3717.358 | 5.01e−20 |
| 11 | 3 | 9 | 10 | 4 | 6 | 3718.141 | 2.93e−21 |
| 9 | 7 | 3 | 9 | 7 | 2 | 3718.468 | 6.41e−22 |
| 9 | 7 | 2 | 9 | 7 | 3 | 3718.468 | 6.41e−22 |
| 11 | 3 | 8 | 11 | 3 | 9 | 3718.865 | 5.71e−22 |
| 4 | 1 | 3 | 3 | 2 | 2 | 3719.231 | 4.78e−20 |
| 4 | 2 | 2 | 5 | 1 | 5 | 3719.300 | 2.80e−20 |
| 6 | 2 | 4 | 6 | 2 | 5 | 3719.846 | 9.53e−21 |
| 7 | 2 | 5 | 6 | 3 | 4 | 3719.889 | 2.17e−20 |
| 11 | 1 | 10 | 10 | 3 | 7 | 3719.979 | 8.08e−23 |
| 9 | 2 | 7 | 10 | 1 | 10 | 3720.385 | 1.52e−21 |
| 2 | 1 | 1 | 2 | 1 | 2 | 3720.445 | 2.51e−20 |
| 5 | 2 | 3 | 6 | 0 | 6 | 3720.612 | 1.32e−22 |
| 9 | 2 | 8 | 8 | 3 | 5 | 3721.537 | 1.10e−20 |
| 10 | 7 | 4 | 10 | 7 | 3 | 3723.159 | 3.31e−22 |
| 10 | 7 | 3 | 10 | 7 | 4 | 3723.159 | 3.31e−21 |
| 7 | 4 | 4 | 8 | 3 | 5 | 3723.377 | 7.36e−21 |
| 2 | 0 | 2 | 1 | 1 | 1 | 3723.493 | 9.64e−20 |
| 2 | 2 | 1 | 3 | 1 | 2 | 3724.080 | 2.42e−20 |
| 5 | 3 | 2 | 6 | 2 | 5 | 3724.242 | 1.99e−20 |
| 7 | 2 | 5 | 7 | 2 | 6 | 3724.560 | 5.33e−21 |
| 3 | 1 | 2 | 3 | 1 | 2 | 3725.053 | 1.51e−20 |
| 7 | 4 | 3 | 8 | 3 | 6 | 3725.511 | 7.34e−21 |
| 3 | 2 | 1 | 4 | 1 | 4 | 3725.722 | 2.86e−20 |
| 10 | 2 | 9 | 9 | 3 | 6 | 3726.797 | 6.77e−21 |
| 9 | 5 | 5 | 10 | 4 | 6 | 3727.181 | 1.71e−21 |
| 4 | 2 | 2 | 5 | 0 | 5 | 3727.190 | 1.44e−22 |
| 10 | 2 | 8 | 11 | 1 | 11 | 3727.394 | 6.52e−22 |

**Continued**

| J' | K'a | K'c | J'' | K''a | K''c | | |
|---|---|---|---|---|---|---|---|
| 9 | 5 | 4 | 10 | 4 | 7 | 3727.680 | 1.71e−21 |
| 1 | 0 | 1 | 0 | 0 | 0 | 3728.112 | 3.83e−20 |
| 7 | 3 | 4 | 8 | 1 | 7 | 3729.425 | 2.69e−23 |
| 11 | 2 | 10 | 10 | 3 | 7 | 3729.787 | 3.67e−21 |
| 11 | 7 | 5 | 11 | 7 | 4 | 3729.968 | 1.63e−22 |
| 11 | 7 | 4 | 11 | 7 | 5 | 3729.968 | 1.63e−22 |
| 8 | 2 | 6 | 8 | 2 | 7 | 3730.828 | 2.98e−21 |
| 4 | 1 | 3 | 4 | 1 | 4 | 3731.141 | 9.50e−21 |
| 4 | 3 | 2 | 5 | 2 | 3 | 3731.549 | 1.80e−20 |
| 11 | 3 | 8 | 10 | 4 | 7 | 3731.999 | 3.12e−21 |
| 1 | 1 | 0 | 1 | 0 | 1 | 3731.349 | 2.71e−19 |
| 2 | 2 | 0 | 3 | 1 | 3 | 3733.700 | 1.85e−20 |
| 5 | 1 | 4 | 4 | 2 | 3 | 3734.058 | 6.69e−20 |
| 2 | 1 | 1 | 2 | 0 | 2 | 3734.957 | 3.84e−19 |
| 4 | 3 | 1 | 5 | 2 | 4 | 3735.287 | 1.75e−20 |
| 8 | 2 | 6 | 7 | 3 | 5 | 3735.852 | 1.98e−20 |
| 3 | 2 | 1 | 4 | 0 | 4 | 3735.929 | 1.07e−22 |
| 3 | 0 | 3 | 2 | 1 | 2 | 3736.011 | 1.89e−16 |
| 6 | 4 | 3 | 7 | 3 | 4 | 3736.954 | 8.09e−21 |
| 2 | 1 | 2 | 1 | 1 | 1 | 3737.204 | 8.04e−20 |
| 3 | 1 | 2 | 3 | 0 | 3 | 3737.557 | 4.21e−19 |
| 6 | 4 | 2 | 7 | 3 | 5 | 3737.943 | 8.08e−21 |
| 10 | 9 | 1 | 11 | 10 | 2 | 3738.286 | 1.49e−23 |
| 10 | 9 | 2 | 11 | 10 | 1 | 3738.286 | 1.49e−23 |
| 9 | 2 | 7 | 9 | 2 | 8 | 3738.589 | 1.51e−21 |
| 5 | 1 | 4 | 5 | 1 | 5 | 3738.631 | 6.07e−21 |
| 2 | 0 | 2 | 1 | 0 | 1 | 3739.483 | 7.26e−20 |
| 8 | 5 | 4 | 9 | 4 | 5 | 3740.514 | 2.27e−21 |
| 2 | 1 | 1 | 1 | 1 | 0 | 3740.524 | 5.01e−20 |
| 8 | 5 | 3 | 9 | 4 | 6 | 3740.731 | 2.27e−21 |
| 4 | 1 | 3 | 4 | 0 | 4 | 3741.348 | 3.91e−19 |
| 1 | 1 | 1 | 0 | 0 | 0 | 3743.343 | 1.92e−19 |
| 6 | 3 | 3 | 7 | 1 | 6 | 3743.732 | 2.61e−23 |
| 3 | 3 | 1 | 4 | 2 | 2 | 3745.083 | 1.01e−20 |
| 2 | 2 | 0 | 3 | 0 | 3 | 3746.205 | 4.39e−23 |
| 5 | 1 | 4 | 5 | 0 | 5 | 3746.522 | 3.18e−19 |
| 3 | 3 | 0 | 4 | 2 | 3 | 3746.720 | 9.99e−21 |
| 10 | 6 | 5 | 11 | 5 | 6 | 3746.854 | 3.67e−22 |
| 10 | 6 | 4 | 11 | 5 | 4 | 3746.897 | 3.67e−22 |
| 6 | 1 | 5 | 6 | 1 | 6 | 3747.392 | 3.86e−21 |
| 3 | 1 | 3 | 2 | 1 | 2 | 3747.680 | 8.08e−20 |

**Table 8. Putting in evidence of the perturbations in the $v_1(v_3)$ band of HTO spectrum.**

| J' | $K'_a$ | $K'_c$ | J'' | $K''_a$ | $K''_c$ | Obs | Cal | Diff |
|---|---|---|---|---|---|---|---|---|
| 8 | 0 | 8 | 9 | 1 | 9 | 3614.632 | 3759.632 | −145 |
| 8 | 0 | 8 | 9 | 0 | 9 | 3616.432 | 3759.432 | −143 |
| 8 | 0 | 8 | 8 | 1 | 7 | 3655.075 | 3821.075 | −166 |
| 8 | 0 | 8 | 7 | 1 | 7 | 3794.388 | 3934.388 | −140 |
| 8 | 0 | 8 | 7 | 0 | 7 | 3598.449 | 3741.449 | −143 |
| 6 | 2 | 5 | 6 | 3 | 4 | 3627.371 | 3303.371 | 324 |
| 6 | 2 | 5 | 7 | 2 | 6 | 3632.055 | 3295.055 | 337 |
| 6 | 2 | 5 | 7 | 1 | 6 | 3661.947 | 3339.947 | 322 |
| 6 | 2 | 5 | 5 | 3 | 5 | 3697.172 | 3390.172 | 307 |
| 6 | 2 | 5 | 6 | 2 | 4 | 3705.219 | 3415.219 | 290 |
| 6 | 2 | 5 | 6 | 1 | 6 | 3779.601 | 3448.601 | 331 |

shows that the closest vibrational state is the state $v_2 = v_3 = 1$ ($v_1 = v_2 = 1$), which energy is estimated to 3739 cm$^{-1}$.

## 3.2. Discussion

The determination of the the dipolar momentum components (**Table 5**) of HTO by the so-called isotopic substitution method allowed us to calculate rays intensities in the $v_1(v_3)$ band.

The experimental rays intensities have not been determined simultaneously with the spectrum record.

For this reason only theoretical values are shown in **Table 7**. In contrast, it should be noted that in the case high excited levels transitions, the calculated energy level has been replaced by its observed value.

In summary, to estimate the quality of the database generated for HTO, there is shown, in **Figure 4**, some of
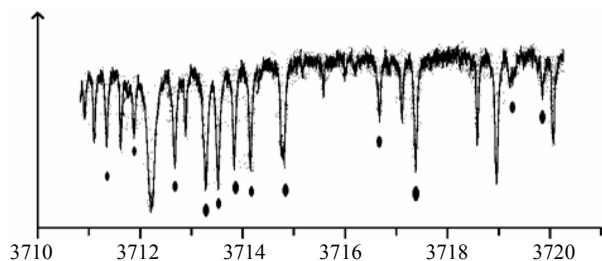
**Figure 4. Spectrum observed (dash) and calculated (point) of the $v_1(v_3)$ band of HTO.**

the observed spectra (dash) and calculated (point). It can be noticed that the results are satisfactory.

## 4. Conclusions

The satisfactory analysis in terms waves rotational numbers of the $v_1(v_3)$ band permitted us to make in evidence a perturbation of the high vibrationnal state. Also, the theoretical calculation of the dipole momentum function allowed us to calculate the non measured intensities of this band's transitions.

Finally, as announced in the introduction, these results permit us to create a HTO spectroscopy database.

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