

# The absorption spectrum of short-lived isotopic variant of water, H<sub>2</sub><sup>15</sup>O: Tentative detection at the Earth's atmosphere

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A calculated *infrared* vibration–rotation spectrum of isotopically modified water, H<sub>2</sub><sup>15</sup>O, is presented. Oxygen-15 has a half-life of about 2 minutes and H<sub>2</sub><sup>15</sup>O may be formed in the atmosphere during thunderstorms as a result of photonuclear processes or when the atmosphere is irradiated by cosmic  $\gamma$ -rays. Variational nuclear motion calculations of vibrational and vibrational-rotational levels up to 25000 cm<sup>-1</sup> and up to  $J = 10$  in angular momentum are performed within the framework of the Born-Oppenheimer approximation using an accurate water potential function. The line shape parameters for H<sub>2</sub><sup>15</sup>O are estimated. Spectral ranges that are promising for the detection of H<sub>2</sub><sup>15</sup>O in the atmosphere are identified and a search for spectral signatures conducted. A spectral feature is tentatively assigned to the 7<sub>52</sub> (0 1 0) and 6<sub>43</sub> (0 0 0) line of H<sub>2</sub><sup>15</sup>O.

**Keywords:** H<sub>2</sub><sup>15</sup>O, spectrum, line list, water vapor, atmospheric FTIR spectra

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## 2. Calculation

We obtain the necessary spectral information for H<sub>2</sub><sup>15</sup>O using two separate methods. The first method is the calculation of vibrational -rotational levels, centers and intensities of spectral lines, based on a high-precision potential energy surface and dipole moment, using the DVR3D package [**Error! Reference source not found.**]. This method uses the Born-Oppenheimer approximation, in which the mass dependence of the potential energy surface is ignored. The second method exploits the fact that the substitution of the oxygen isotope

refers to the case of substitution of heavy atoms. In this case, a small parameter appears in the problem, namely the relative change in mass during isotope substitution. The application of perturbation theory makes it possible to represent the isotopic shift of an individual level in the form of a series in powers of  $\mu = (m' - m)/m'$ , where  $m'$  and  $m$  are the masses of the substituting and substituted isotopes, respectively. In this case it is possible, using the experimental values of the levels of the stable isotopologues  $H_2^XO$  ( $X = 16, 17, 18$ ) from the list of empirical levels provided by a IUPAC task group [Error! Reference source not found., Error! Reference source not found., 28], to determine the coefficients of the second-degree interpolating polynomial and to extrapolate the energy, determining the values of the levels for  $X = 15$ .

For these calculations we take the oxygen isotope masses from [8]: 15.0030656 Da for oxygen-15, and 15.99491461960, 16.9991317566, 17.9991596128 Da for  $^{16}O$ ,  $^{17}O$ ,  $^{18}O$ , respectively. In this case, the parameters  $\mu$  are equal -0.0661097569019, 0.0590746134202, and 0.1113521428953 for  $^{15}O$ ,  $^{17}O$ ,  $^{18}O$ .

To estimate vibration energy levels of  $H_2^{15}O$ , we have used energy levels  $H_2^{16}O$ ,  $H_2^{17}O$  and  $H_2^{18}O$  from [28]. After that, for each level a set of linear equations:

$$\begin{aligned} {}^{17}E_v - {}^{16}E_v &= x_1^v \mu(16 \rightarrow 17) + x_2^v \mu(16 \rightarrow 17)^2 \\ {}^{18}E_v - {}^{16}E_v &= x_1^v \mu(16 \rightarrow 18) + x_2^v \mu(16 \rightarrow 18)^2 \end{aligned}$$

has been solved giving  $x_1^v$  and  $x_2^v$ . The energy levels of  $^{15}O$  isotopic variant were calculated using formula:

$${}^{15}E_v = {}^{16}E_v + x_1^v \mu(16 \rightarrow 15) + x_2^v (\mu(16 \rightarrow 15))^2$$

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