Theoretical line list of $D_2\,^{16}O$ up to $16{,}000\,cm^{-1}$ with an accuracy close to experimental

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Abstract

A line list for $D_2\,^{16}O$ isotopologue of water molecule was calculated in the region 0–$16{,}000\,cm^{-1}$ with energy levels up to $J = 30$. Variational calculations are based on the semi-theoretical potential energy surface obtained by morphing *ab initio* potential using the experimental energy levels of $D_2\,^{16}O$. For energy levels with $J = 0, 2, 5$ and 10, the standard deviation of the fit is $0.023\,cm^{-1}$. This line list should make an excellent starting point for spectroscopic modeling and analysis of D_2O rovibrational spectra.
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1. Introduction

Due to the fundamental importance of water and the many applications of its spectra, the development of a complete global theoretical model of the vibration–rotation spectra of water molecule is one of the major tasks of molecular spectroscopy. Despite the apparent simplicity of the water molecule, more than half a century of research with effective Hamiltonian models can only describe its spectra with experimental accuracy in limited frequency regions for a small number of vibrational states. Any attempt to describe all energy levels in the electronic ground state, using effective Hamiltonians, will lead to a drastic increase in the number of parameters required for the optimization of the model using experimental data. Such a procedure does not look feasible in spite of leaving aside the problem of dark vibrational states for which direct experimental information is unavailable.

The problem could be solved by variational calculations, that allow the calculation of global theoretical spectra. The quality of such calculations is primarily determined by the potential energy surface (PES). But when trying to achieve accuracy close to the experimental, it is necessary to consider small physical effects that are not usually included in the standard treatment of molecular dynamics in the Born–Oppenheimer (BO) approximation. The relativistic and quantum electrodynamics effects, used to obtain the accurate *ab initio* PES [1,2], are not dependent on nuclear masses and are the same for all isotopologues of water. The adiabatic and

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nonadiabatic corrections to BO approximation on the other hand are mass dependent. The nonadiabatic correction, which accounts for the influence of the excited electronic states on the energy levels in the ground electronic state, is very difficult to treat quantitatively. It is important to have experimental values for the energy levels of different water isotopologues in order to improve the theory of mass-dependent corrections to the BO approximation.

The spectroscopically determined PESs of the $H_2{}^{16}O$, $H_2{}^{17}O$ and $H_2{}^{18}O$ isotopologues of water were obtained in our previous work [3]. Using these PESs we have calculated theoretical line lists for these molecules in the range 0–26,000 cm^{-1} with J values up to 10 [3,4]. In this work we continue the study of water molecule isotopologues spectra by calculating the line list of D_2O in the 0–16,000 cm^{-1} range with J values up to 30.

2. Fit of the PES

One of the main sources of new energy levels for the water molecule are hot spectra with temperatures 1800–3000 K [5,6]. In our recent papers on analysis of the hot ($T = 1800$ K) laboratory emission FT spectra of D_2O in the region 380–4750 cm^{-1} [6,7], more than 5800 new energy levels were determined. The analysis in [6,7] was performed with the aid of semi-theoretical PES determined using experimental D_2O energy levels from previous works [8–17] and from our study of the hot spectra in the 380–1877 cm^{-1} region [7]. The starting point for the fit of that work was high-quality *ab initio* PES [1], obtained using 346 MRCI electronic energies calculated at different nuclei geometries (*ab initio* points) and different corrections to BO approximation. The standard deviation of energy levels calculated using an *ab initio* PES for almost all previously known 17,795 energy levels of the five water isotopologues ($H_2{}^{16}O$, $H_2{}^{17}O$, $HD^{18}O$, $HD^{16}O$, $D_2{}^{16}O$) was less than 1 cm^{-1}. To obtain the accuracy of calculated levels close to the experimental, we slightly distort the original *ab initio* PES multiplying it by morphing function [18], the parameters of which are then optimized using experimental energy levels. In [7] this procedure was applied to get obtain fitted potential of $D_2{}^{16}O$. The standard deviation for 620 experimental energy levels of D_2O with $J = 0, 2, 5$ and 10 was 0.033 cm^{-1}.

Since the publication of paper [7], there has been a significant progress in the study of water spectra [2,5,6]. New energy levels for D_2O were determined in analysis of hot ($T = 1800$ K) and cold ($T = 296$ K) spectra [6,19–22]. The number of vibrational states studied by the experiment was increased by 19. To improve the quality of *ab initio* PES, 1149 new *ab initio* points were calculated [2]. These new electronic energies, in conjunction with the old ones [1], provided us with a new starting point [23] for the fitting procedure. From this starting point [23], a number of fits were performed. Our final fit included all data for states with $J = 0, 2, 5$ and 10. It is both computationally expensive and unnecessary to perform fits for all rotational energy levels simultaneously. This constituted over 1160 energy levels including new experimental data, some of which are not yet published [22]. From these, about 20 levels were excluded on the grounds that they had an unacceptably large error. It is likely that some of these levels actually result from misassigned transitions. All data were included in the fits with the same weight without considering their experimental accuracy.

We performed several calculations with different morphing functions and have chosen the optimal set of parameters:

$$V_{\text{fit}}(r_1, r_2, \theta) = f_{\text{morp}}(r_1, r_2, \theta) V_{\text{ab initio}}(r_1, r_2, \theta). \tag{1}$$

For our fits, the morphing function was expressed as a power series in the so-called Jensen coordinates:

$$s_1 = \frac{r_1 + r_2}{2} - r_e,$$
$$s_2 = \cos \theta - \cos \theta_e,$$
$$s_3 = \frac{r_1 - r_2}{2}. \tag{2}$$

$$f_{\text{morp}} = c_{000} + \sum_{ijk} c_{ijk} s_1^i s_2^j |s_3^k|; \ 2 \leqslant i + j + k \leqslant N. \tag{3}$$

In particular, we tested all fourth-order ($N = 4$) terms as well as the effect of including fifth-order ($N = 5$) terms. Optimization of 27 parameters of the morphing function using the set of all known experimental levels with $J = 0, 2, 5$ and 10 allowed us to obtain the standard deviation for the fitted levels $0.023\,\mathrm{cm}^{-1}$. The constants of the morphing function used to determine the fitted potential are given in Table 1. Note that due to symmetry considerations, only even numbers of k were included in the fit.

This standard deviation ($0.023\,\mathrm{cm}^{-1}$) is better by one third than our previous result even though the number of fitted levels was almost doubled. The achieved theoretical accuracy is very close to the experimental one, for which weaker lines could be estimated within 0.01–$0.02\,\mathrm{cm}^{-1}$. Table 3 shows comparison between our calculations and all known experimental band origins. Although our fits only used data for $J = 0, 2, 5$ and 10, they reproduce the data for states with $J \leqslant 10$ in a uniform fashion. This suggests that our decision not to fit all these J states simultaneously did not lead to a loss of accuracy.

All our calculations were carried out using the program suite DVR3D [24], in Radau coordinates. During the fitting procedure, 29 radial grid points and 40 angular grid points were used. Vibrational Hamiltonian matrices of final dimension 1500 were diagonalized and for the rotational problems these matrices had dimension $300 \times (J + 1 - p)$, where J is the total angular momentum quantum number and p—the parity. Nuclear masses have been used for all calculations.

Rotational nonadiabatic effects increase approximately as J^2 [25], and it is necessary to consider them for calculations with higher J. Schwenke [26] calculated simplified, effective nonadiabatic operators for the estimation of the nonadiabatic correction. These operators have been shown to work well [27]. The values of these three rotational nonadiabatic operators were treated as parameters, which were determined by the condition that provides the best prediction of energy levels with $J = 20$ and 30. The best results were obtained by multiplying the values given by Schwenke by -0.08 (minus 8%). The standard deviation of the

Table 1
Fitted coefficients, $c_{i,\,j,k}$, of the morphing function

i	j	k	
0	0	0	1.000315626194052
1	1	0	0.006897717102802
2	0	0	0.003446617478693
3	0	0	−0.008075277875726
0	0	2	0.004207336693463
4	0	0	−0.012592391764251
0	2	0	−0.003482433322662
0	3	0	−0.001358016080131
0	4	0	0.006631312740722
2	1	0	0.002223707033554
1	2	0	0.007907994828571
1	0	2	−0.015424047003807
0	1	2	0.007034912608434
0	0	4	−0.009306891128230
3	1	0	−0.017426966436679
1	3	0	−0.024772110218175
2	2	0	0.006656114951179
2	0	2	0.070807268033961
1	1	2	−0.013481961720405
0	2	2	0.001875271464578
5	0	0	0.036075242515179
0	5	0	0.004524925820457
4	1	0	−0.022902545574679
3	0	2	−0.041562757562605
2	3	0	−0.008614083413760
1	4	0	−0.009596605976173
1	0	4	−0.057345237497490

Dimensions are $a_0^{-(i+k)}$.

experimental levels predicted with the rotational nonadiabatic correction is $0.05\,\mathrm{cm}^{-1}$ for 392 levels with $J = 20$ and $0.08\,\mathrm{cm}^{-1}$ for 163 levels with $J = 30$. The fitted potential thus preserves its high quality at high J values. All further calculations presented in this paper use these scaled nonadiabatic operators.

As it has been discussed in our previous paper [3], the true magnitude of nonadiabatic corrections to rovibrational levels using PESs remains uncertain. The quality of predictions for high J levels certainly depends on rotational nonadiabatic effects, but it appears impossible to determine these effects purely by fitting.

3. Line list calculation

To facilitate the analysis of new experimental spectra of D_2O, we have calculated a line list for transitions in the 0–$16,000\,\mathrm{cm}^{-1}$ range with J values up to 30 at temperature 296 K using the program suite DVR3D [24]. The intensity cut off $1.0 \times 10^{-30}\,\mathrm{cm\,molecule}^{-1}$ was used, which should be enough for analyzing D_2O experimental spectra. During the line list calculations, we used 40 angular grid points and reduced the radial grid of 25 points to save computer time; this was found to give only negligible differences for the energy range considered here. Vibrational Hamiltonian matrices of final dimension 1500 were diagonalized. For the rotational problems these matrices had dimension $250 \times (J + 1 - p)$.

Table 2
Internal partition function of D_2O obtained using calculated energy levels Q_c (this work) and experimental ones Q_e (work [28]) of D_2O at different temperatures (T)

T (K)	Q_c	Q_e
1	1.9999	2.0001
5	2.2015	2.1141
10	3.5201	3.0432
20	7.9007	6.7353
30	13.4695	11.7786
40	19.9372	17.7607
50	27.1827	24.5271
60	35.1258	31.9917
70	43.7073	40.0944
80	52.8809	48.7893
90	62.6097	58.0392
100	72.8628	67.8129
150	131.195	123.747
200	199.882	190.028
300	364.368	349.650
400	564.083	544.299
500	801.899	776.679
600	1082.773	1051.467
700	1412.964	1374.267
800	1799.846	1751.004
900	2251.697	2187.318
1000	2777.557	2688.09
1500	6871.18	
2000	14,437.22	
2500	26,964.67	
3000	45,796.43	
3500	71,826.51	
4000	105,361.9	
4500	146,174.6	
5000	193,651.2	
5500	246,954.6	
6000	305,155.7	

In [28] the partition functions of HDO and D_2O molecules were calculated using compilations of the then known experimental levels. For D_2O it included 5638 levels. We have calculated more than 100,000 levels with $J = 0$–30 and up to energies slightly higher than $16,000\,cm^{-1}$. We have used statistical weights 1 and 2 for para and ortho states of D_2O, so our values differ by a factor of 3 from the values in [28]. The results of the partition function calculations are presented in Table 2 with the values from the previous study. We have multiplied the values from [28] by a factor of 3 for easier comparison. At temperature 300 K our values for the partition function are about 4% higher. As we have included considerably more energy levels in the calculation of the partition function, our partition function should be more complete than in paper [28]. The increase of the number of energy levels included in the partition function calculations from about 6000 [28] to more than 100,000 in this paper changed the value of the partition function only by 4% for $T = 1000$ K. We believe that the inclusion of all bound levels of D_2O molecule with energies higher than $16,000\,cm^{-1}$ could possibly increase the Q value only by several percent even at temperature 6000 K.

For the intensity calculations, we used the dipole moment surface of Schwenke and Partridge [29]. We have calculated the line list at 296 K. Knowing the values of the partition function and the energy of the transition's lower state, which is included in the line list (see Table 5), it is possible to recalculate the line intensities to any other temperature.

4. Labeling of energy levels

The energy levels of D_2O, calculated by the DVR3D program suite [24], are automatically assigned with only rigorous quantum numbers, J, p (rotational parity), ortho/para. The labeling of the levels with the generally used harmonic oscillator and rigid rotor quantum numbers v_1, v_2, v_3, J, K_a and K_c was made using the algorithm of paper [30], used in [4,7]. This method is based on the smooth dependence of a levels energy upon vibrational and rotational quantum numbers. It also takes into account the supposedly correct labeling of experimentally determined levels. Vibrational labeling of levels with $J = 0$ was checked by analyzing the numerical wave functions [4,31]. In Table 3 we present the calculated band origins of D_2O up to $16,000\,cm^{-1}$. Small differences between observed and calculated values show good quality of the calculations.

Table 3
Calculated band origins of D_2O

v_1	v_2	v_3	$E_{calc.}$	$E_{obs.} - E_{calc.}$
0	1	0	1178.448	0.069
0	2	0	2336.884	0.045
1	0	0	2671.637	−0.008
0	0	1	2787.711	−0.007
0	3	0	3474.323	0.004
1	1	0	3841.430	
0	1	1	3956.042	0.029
0	4	0	4589.274	
1	2	0	4990.804	−0.023
0	2	1	5105.380	−0.005
2	0	0	5291.734	0.011
1	0	1	5373.914	0.011
0	0	2	5529.444	0.006
0	5	0	5679.583	
1	3	0	6119.021	
0	3	1	6235.059	−0.023
2	1	0	6452.970	−0.010
1	1	1	6533.256	0.020
0	1	2	6687.011	0.018
0	6	0	6742.106	
1	4	0	7224.686	
0	4	1	7343.929	
2	2	0	7593.248	

Table 3 (*continued*)

v_1	v_2	v_3	$E_{\text{calc.}}$	$E_{\text{obs.}} - E_{\text{calc.}}$
1	2	1	7672.919	−0.014
0	7	0	7771.948	
0	2	2	7826.283	
3	0	0	7852.948	0.020
2	0	1	7899.832	0.006
1	0	2	8054.093	
0	0	3	8220.196	0.018
1	5	0	8305.537	
0	5	1	8430.285	
2	3	0	8712.060	
0	8	0	8760.674	
1	3	1	8792.665	
0	3	2	8947.015	
3	1	0	9005.495	
2	1	1	9050.349	0.000
1	1	2	9202.706	−0.010
1	6	0	9357.488	
0	1	3	9366.317	0.004
0	6	1	9491.641	
0	9	0	9691.297	
2	4	0	9808.987	
1	4	1	9891.553	
0	4	2	10,048.288	
3	2	0	10,136.341	
2	2	1	10,180.111	
1	2	2	10,330.597	
4	0	0	10,341.021	
3	0	1	10,358.547	−0.012
1	7	0	10,368.760	
0	2	3	10,494.837	
0	7	1	10,524.245	
2	0	2	10,538.484	
0	10	0	10,553.561	
1	0	3	10,679.697	
0	0	4	10,861.135	
2	5	0	10,880.831	
1	5	1	10,967.959	
0	5	2	11,128.717	
3	3	0	11,245.683	
2	3	1	11,289.721	
1	8	0	11,295.354	
0	11	0	11,433.488	
1	3	2	11,441.212	
4	1	0	11,483.656	−0.017
3	1	1	11,500.241	0.007
0	8	1	11,521.903	
0	3	3	11,605.758	0.032
2	1	2	11,679.272	0.117
1	1	3	11,816.585	0.052
2	6	0	11,923.863	
0	1	4	11,995.186	0.052
1	6	1	12,019.191	
0	6	2	12,184.257	
1	9	0	12,196.878	
3	4	0	12,332.356	
0	12	0	12,364.325	
2	4	1	12,378.446	
0	9	1	12,473.122	

Table 3 (*continued*)

v_1	v_2	v_3	$E_{calc.}$	$E_{obs.} - E_{calc.}$
1	4	2	12,530.773	
4	2	0	12,603.546	
3	2	1	12,618.921	0.009
0	4	3	12,698.520	
5	0	0	12,737.416	
4	0	1	12,743.027	0.009
2	2	2	12,799.139	
2	7	0	12,926.072	
1	2	3	12,934.102	
3	0	2	12,988.318	
1	7	1	13,039.942	
2	0	3	13,088.189	
0	2	4	13,112.050	
1	10	0	13,126.745	
0	7	2	13,218.997	
1	0	4	13,263.805	
0	13	0	13,283.311	
0	0	1	13,357.575	
3	5	0	13,398.051	
2	5	1	13,446.273	
0	0	5	13,452.009	
1	5	2	13,599.156	
4	3	0	13,702.639	
3	3	1	13,717.384	
0	5	3	13,772.169	
2	8	0	13,855.919	
5	1	0	13,869.375	
4	1	1	13,876.046	
2	3	2	13,900.319	
1	8	1	14,014.450	
1	3	3	14,033.359	
1	11	0	14,038.636	
3	1	2	14,121.740	
0	11	1	14,191.879	
0	3	4	14,212.143	
2	1	3	14,216.683	
0	8	2	14,221.800	
0	14	0	14,276.776	
1	1	4	14,388.784	
3	6	0	14,434.125	
2	6	1	14,488.312	
0	1	5	14,573.340	
1	6	2	14,643.386	
2	9	0	14,753.156	
4	4	0	14,782.056	
3	4	1	14,794.877	
0	6	3	14,825.401	
1	9	1	14,924.347	
2	4	2	14,961.964	
1	12	0	14,970.584	
4	2	1	14,979.282	
5	2	0	14,986.609	
6	0	0	15,049.996	
5	0	1	15,051.338	
0	12	1	15,074.385	
1	4	3	15,113.805	
0	9	2	15,185.864	
3	2	2	15,231.378	

Table 3 (continued)

v_1	v_2	v_3	$E_{calc.}$	$E_{obs.} - E_{calc.}$
0	4	4	15,295.265	
2	2	3	15,322.836	
0	15	0	15,345.864	
4	0	2	15,388.749	
3	7	0	15,433.304	
3	0	3	15,441.861	
1	2	4	15,494.245	
2	7	1	15,500.814	
2	0	4	15,624.868	
1	7	2	15,649.098	
0	2	5	15,677.610	
2	10	0	15,692.517	
1	0	5	15,798.422	
1	10	1	15,820.486	
4	5	0	15,836.958	
0	7	3	15,854.312	
3	5	1	15,861.109	
1	13	0	15,896.481	
0	13	1	15,992.380	
0	0	6	15,993.468	
2	5	2	16,026.806	
4	3	1	16,065.404	
5	3	0	16,066.898	

Table 4
An example transition from the theoretical line list of $D_2^{16}O$

Number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26
Value	0	14	1	9	15	1	1	2683.70	2683.40	0.306822	0.50E−00	0.119E−29	0.259E−10	0.157E−09	14	13	1	0	0	0	15	12	4	0	0	0

It should be noted here that our labeling procedure, as with all methods of 'determining' approximate quantum numbers, is not free from error. When the line list is used during the assignment of experimental spectra, other factors should also be taken into account, for example, the dependence of the transition intensities on the quantum numbers.

In Table 4 we present a sample of our calculated line list. Table 5 explains the output format. The line list is available for downloads from the URL address: http://saga.atmos.appl.sci-nnov.ru/d2o/ or from the authors.

5. Conclusions

We present a theoretical line list for $D_2^{16}O$ isotopologue of the water molecule. The line list is calculated within the range 0–16,000 cm^{-1}, with J values up to 30 at temperature 296 K. The line list is based on a semi-theoretical PES determined by fitting *ab initio* PES [23] to experimental energy levels. The standard deviation of the fitted levels with $J = 0, 2, 5$ and 10 is 0.023 cm^{-1}. All variational calculations were performed using the program suite DVR3D [24].

Our previous semi-theoretical D_2O line list [7] was a very useful tool for analyzing experimental spectra, especially for assigning high-temperature ($T = 1800$ K) transitions with J up to 30 [6,7]. However, it had some limitations when applied to the room-temperature spectrum for frequencies higher than 9000 cm^{-1} [19]. The old line list was based on a PES obtained from fitting a set of energy level with only two vibrational states with energies higher than 9000 cm^{-1}. The new set of experimental energy level has 20 vibrational states in the region 9000–14,000 cm^{-1}. The accuracy of our new line list is significantly higher in this region and has already been

Table 5
Explanation of the theoretical line list format

Column number	Explanation of column's content
1	Level's vibration symmetry: 0—symmetric states, 1—symmetric states
2	Upper level quantum number J
3	Upper level rotation symmetry (0 or 1)
4	Upper level number in current block
5	Lower level quantum number J
6	Lower level rotation symmetry (0 or 1)
7	Lower level number in current block
8	Upper level energy value (cm^{-1})
9	Lower level energy value (cm^{-1})
10	Transition frequency (cm^{-1})
11	Squared transition dipole moment (D^2)
12	Absolute line intensity, shows absorption by one molecule (cm molecules^{-1})
13	Relative transition intensity (normalized by the maximum transition intensity)
14	Einstein's coefficient (s^{-1})
15	Upper level quantum number J
16	Upper level quantum number K_a
17	Upper level quantum number K_c
18	Upper level quantum number v_1
19	Upper level quantum number v_2
20	Upper level quantum number v_3
21	Lower level quantum number J
22	Lower level quantum number K_a
23	Lower level quantum number K_c
24	Lower level quantum number v_1
25	Lower level quantum number v_2
26	Lower level quantum number v_3

successfully used for study of intracavity laser absorption spectra of D_2O between 11,400 and 11,900 cm^{-1} [21]. Therefore, our new calculated line list should make an excellent starting point for spectroscopic modeling and currently is the best available for the analysis of $D_2\,^{16}O$ experimental spectra.

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