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Rotational and Centrifugal Parameters of $H_2{}^{17}O$ and $H_2{}^{18}O$ (010) States

We report here the results of solving the inverse problem for the (010) states of the molecules $H_2{}^{17}O$ and $H_2{}^{18}O$ which are of interest for some applied problems of water vapor spectroscopy, in particular, for analyzing the hot bands.

The rotational and centrifugal constants of the (010) states for the molecules $H_2{}^{17}O$ and $H_2{}^{18}O$ have been given in Ref. (*1*). However, it appears that the parameters given in Ref. (*1*) can be improved. In particular, contrary to expectations, some parameters of $H_2{}^{17}O$ and $H_2{}^{18}O$ (e.g., δ_K, H_{KJ}, H_{JK}, H_J, h_K, h_{JK}) differ for these two isotope species and in comparison with $H_2{}^{16}O$ species (*2*). Therefore, in this note we once again consider the problem of determining the (010)-state parameters of the molecules $H_2{}^{17}O$ and $H_2{}^{18}O$ based on precise line centers of the ν_2 bands (*3*) as well as on the energy levels of the (000) states from Ref. (*4*). The energy levels (E^i_{exp}) for the (010) states obtained from the experimental data are presented in Table I.

The data from Table I were used as initial information in determining the rotational and centrifugal distortion constants. Making use of the known (010)-state constants of the $H_2{}^{16}O$ molecule (*2*) and simple and sufficiently accurate isotopic relations (*5*) for the rotational and centrifugal constants, the parameters at large orders of the J_α operators in the Watson's Hamiltonian (*6*) were determined. They are presented in columns 2 and 4 of Table II without confidence intervals. The remaining parameters were determined by fitting the results of calculations to the experimental data (the initial approximations for these parameters were also determined using the isotopic relations and are given in columns 3 and 5 of Table II). The parameters thus obtained and the 95% confidence intervals for them are given in Table II. As an illustration of the correctness of the obtained parameters, Table I gives the values $\Delta = (E^i_{calc} - E^i_{exp}) \times 10^4$ cm^{-1} for energy levels. It is seen that the parameters from Table II allow the energy levels to be reproduced with an accuracy close to the experimental values. In this case for 90 initial levels of the $H_2{}^{18}O$ molecule the following condition is fulfilled:

$$0 \times 10^{-3} \leqslant |\Delta| < 2 \times 10^{-3} \text{ cm}^{-1} \quad 64.5\% \text{ levels},$$

$$2 \times 10^{-3} \leqslant |\Delta| < 4 \times 10^{-3} \text{ cm}^{-1} \quad 27.8\%,$$

$$4 \times 10^{-3} \leqslant |\Delta| < 6 \times 10^{-3} \text{ cm}^{-1} \quad 4.4\%,$$

$$6 \times 10^{-3} \leqslant |\Delta| < 9 \times 10^{-3} \text{ cm}^{-1} \quad 3.3\%.$$

Similarly, for 71 levels of the $H_2{}^{17}O$ molecule,

$$0 \times 10^{-3} \leqslant |\Delta| < 1 \times 10^{-3} \text{ cm}^{-1} \quad 71.9\% \text{ levels},$$

$$1 \times 10^{-3} \leqslant |\Delta| < 2 \times 10^{-3} \text{ cm}^{-1} \quad 21.1\%,$$

$$2 \times 10^{-3} \leqslant |\Delta| < 3 \times 10^{-3} \text{ cm}^{-1} \quad 5.6\%,$$

$$3 \times 10^{-3} \leqslant |\Delta| < 5 \times 10^{-3} \text{ cm}^{-1} \quad 1.4\%.$$

One more additional criterion of correctness of the obtained parameters is their satisfactory agreement with the ones predicted on the basis of isotopic relations.

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TABLE I

Energy Levels for the States (010) of $H_2{}^{17}O$ and $H_2{}^{18}O$

			$H_2{}^{18}O$		$H_2{}^{17}O$					$H_2{}^{18}O$		$H_2{}^{17}O$	
J	K_A	K_C	$E_{exp.}$	Δ	$E_{exp.}$	Δ	J	K_A	K_C	$E_{exp.}$	Δ	$E_{exp.}$	Δ
0	0	0	1588.2760	16	-	-	6	5	2	2536.9095	-45	2544.4091	21
1	0	1	1612.0495	-17	1615.1150	- 1	6	5	1	2536.9352	-49	2544.4327	25
1	1	1	1628.0594	15	1631.3150	3	6	6	1	2714.4427	21	2723.6295	- 1
1	1	0	1633.6363	- 9	1636.8738	- 8	6	6	0	2714.4427	24	2723.6195	2
2	0	2	1658.3346	12	1661.4592	- 2	7	0	7	2171.7396	8	2175.9365	10
2	1	2	1670.0376	- 2	1673.3475	- 8	7	1	7	2172.1432	-11	2176.3594	3
2	1	1	1686.7325	9	1689.9924	- 2	7	1	6	2300.7733	11	2305.0021	-19
2	2	1	1734.2207	-16	1738.0274	14	7	2	6	2308.9059	-22	2313.4449	0
2	2	0	1735.4382	0	1739.2284	12	7	2	5	2384.0413	26	2388.0712	- 1
3	0	3	1725.0177	5	1728.2596	0	7	3	5	2429.1341	25	2434.2280	7
3	1	3	1732.2625	1	1735.6652	- 9	7	3	4	2453.0571	30	2457.6748	- 9
3	1	2	1765.3991	-11	1768.7036	- 4	7	4	4	2556.4627	11	-	-
3	2	2	1805.5770	-21	1809.4435	0	7	4	3	2559.3135	38	2565.3441	26
3	2	1	1811.2915	-27	1815.0784	- 2	7	5	3	2707.9219	-32	-	-
3	3	1	1897.4525	41	1902.1590	17	7	5	2	2708.0617	-20	2715.6400	- 6
3	3	0	1897.6283	27	1902.3285	18	7	6	2	2885.7189	-16	-	-
4	0	4	1810.1881	13	1813.6109	5	7	6	1	2885.7202	4	-	-
4	1	4	1814.0867	1	1817.6253	- 8	7	7	1	3086.1884	- 3	-	-
4	1	3	1868.2539	7	1871.6541	3	7	7	0	3086.1884	- 3	-	-
4	2	3	1899.6093	-36	1903.5683	- 9	8	0	8	2327.8832	5	2332.4050	-41
4	2	2	1914.8807	-21	1918.6568	- 8	8	1	8	2328.0644	- 2	2332.5908	8
4	3	2	1994.7036	-11	1999.4624	0	8	1	7	2480.5031	0	2485.1500	12
4	3	1	1995.8700	- 8	2000.5979	- 2	8	2	7	2484.8743	4	2489.7253	0
4	4	1	2117.0093	34	2122.9318	-16	8	2	6	2586.6329	-10	-	-
4	4	0	2117.0287	52	2122.9517	-11	8	3	6	2618.9198	66	2624.2283	- 1
5	0	5	1913.0228	14	1916.6723	7	8	3	5	2661.0026	33	-	-
5	1	5	1914.9335	- 4	1918.6535	- 4	8	4	5	2751.4170	84	2757.6641	- 2
5	1	4	1993.2766	21	1996.8525	16	8	5	4	2903.3290	27	-	-
5	2	4	2015.4540	-35	2019.5506	- 7	8	6	3	3081.2002	- 3	-	-
5	2	3	2045.9224	- 6	2049.7109	- 2	9	0	9	2501.9532	38	2506.8255	11
5	3	3	2116.1385	-27	2120.9713	- 5	9	1	9	2502.0382	1	2506.9119	11
5	3	2	2120.4547	-27	2125.1780	-11	9	1	8	2677.2812	-32	2682.3744	- 1
5	4	2	2238.9740	- 2	2244.9584	-13	9	2	8	2679.5309	- 7	2684.7462	- 6
5	4	1	2239.1574	-15	2245.1332	-11	9	2	7	2808.2784	-70	-	-
5	5	1	2390.3545	-17	2397.7783	- 5	9	4	6	2969.7327	-15	-	-
5	5	0	2390.3557	- 5	2397.7805	- 4	10	0	10	2693.9534	2	2699.2077	8
6	0	6	2033.4890	4	2037.3966	9	10	1	10	2693.9917	-10	2699.2473	7
6	1	6	2034.3763	0	2038.3239	- 1	10	1	9	2891.3557	-33	-	-
6	1	5	2138.0884	19	2141.9432	24	10	2	9	2892.4892	-18	2898.1181	1
6	2	5	2152.1814	-22	2156.4702	- 1	10	2	8	3047.0763	- 2	-	-
6	2	4	2202.9924	18	2206.8538	5	11	0	11	2903.8453	-35	2909.5148	- 1
6	3	4	2261.2172	-13	2266.1567	2	11	1	11	2903.8603	-13	-	-
6	3	3	2272.6457	- 3	2277.3226	- 2	11	2	10	3123.5012	- 1	-	-
6	4	3	2385.5128	-12	2391.5661	2	12	1	12	3131.5829	9	-	-
6	4	2	2386.3657	-13	2392.3853	8	12	2	11	3372.4158	-12	-	-

TABLE II

Rotational and Centrifugal Parameters for the States (010) of $H_2{}^{17}O$ and $H_2{}^{18}O$

	$H_2{}^{18}O$		$H_2{}^{17}O$	
1	2	3	4	5
	1588.27756(224)	1588	1591.32584(122)	1592
A	30.729085(993)	30.712	30.918292(570)	30.921
B	14.684494(316)	14.689	14.685687(169)	14.688
C	9.091301(175)	9.092	9.108943(106)	9.111
$10_{-2}\,\Delta_K$	5.62144(931)	5.59	5.73413(754)	5.67
$10_{-3}\,\Delta_{JK}$	-7.5345(498)	-7.43	-7.6368(134)	-7.52
$10_{-3}\,\Delta_J$	1.39154(331)	1.38	1.39091(186)	1.39
$10_{-3}\,\delta_K$	3.5882(257)	3.67	3.68550(570)	3.72
$10_{-4}\,\delta_J$	5.7684(226)	5.77	5.78577(966)	5.78
$10_{-4}\,H_K$	3.5701(366)	3.41	3.7630(362)	3.47
$10_{-5}\,H_{KJ}$	-5.050(301)	-4.34	-4.9217(544)	-4.42
$10_{-6}\,H_{JK}$	4.367(294)	3.3	3.6	
$10_{-7}\,H_J$	5.775(240)	6.19	5.6968(832)	6.15
$10_{-5}\,h_K$	8.055(337)	8.06	8.6212(578)	8.24
$10_{-7}\,h_J$	2.768(150)	2.93	2.92	
$10_{-6}\,L_K$	-2.2244(500)	-1.91	-2.4780(512)	-2.05
$10_{-7}\,L_{KKJ}$	1.056(518)	0.59	0.70	
$10_{-7}\,l_K$	-3.292(610)	-4.08	-4.19	
$10_{-9}\,l_{JK}$	3.2		-	
$10_{-8}\,P_K$	1.01		1.03	
$10_{-10}\,P_K$	8.28		8.6	
$10_{-11}\,Q_K$	-3.03		-3.09	
$10_{-14}\,R_K$	3.8		-	

Values in the Parentheses are 26 confidence intervals

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