One-Dimensional Approximation of the Effective Rotational Hamiltonian of the Ground State of the Water Molecule

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A method is presented for summation of the divergent perturbation-theory series used in molecular spectroscopy, by means of a one-dimensional approximation. Application of the proposed method enables one to fit the energy levels of the ground state of the water molecule (Mol. Phys. *32*, 499–521 (1976)) to a maximum difference between the observed and the calculated levels of less than 8 cm^{-1} for levels with the maximum rotational quantum numbers $K = 20$ and $J = 20$ in a model with 24 parameters and terms up to J^8. © 1985 Academic Press, Inc.

INTRODUCTION

A method of summation of the divergent series arising from the perturbation theory used in molecular spectroscopy, by means of a one-dimensional approximation, is presented. The application of the proposed method enables one to fit the energy levels of the ground state of the water molecule (*1*) to a maximum difference between observed and calculated levels of less than 8 cm^{-1} for levels with the maximum rotational quantum numbers $K = 20$ and $J = 20$ in a model of 24 parameters and terms up to J^8. Thus, a smaller difference between observed and calculated levels is obtained by a smaller number of constants and powers of the angular momentum than in the conventional fitting of Ref. (*2*) by a simple rearrangement of the conventional perturbation terms.

In the first part of the paper the use of such methods is validated; some details of the proposed method are presented in the second part and the results of the fitting of the H$_2^{16}$O ground state energy levels are given in the third part.

PART I

The use of the perturbation theory for the calculation of molecular energy levels results in an effective rotational Hamiltonian in Watson's form (for asymmetric tops):

$$H = H_{\text{diag}}^{(2N)} + \frac{1}{2} H_{\text{nondiag}}^{(2N)}(J_x^2 - J_y^2) + \frac{1}{2} (J_x^2 - J_y^2)H_{\text{nondiag}}^{(2N)},$$

$$H_{\text{diag}}^{(8)} = C_0 + C_1 + C_2 + C_3,$$

$$H_{\text{nondiag}}^{(8)} = b_0 + b_1 + b_2 + b_3,$$

$$C_0 = \left(A - \frac{B + C}{2}\right)J_z^2 + \frac{B + C}{2} J^2,$$

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$$C_1 = -\Delta_J J^4 - \Delta_{JK} J^2 J_z^2 - \Delta_K J_z^4,$$

$$C_2 = H_J J^6 + H_{JK} J^4 J_z^2 + H_{KJ} J^2 J_z^4 + H_K J_z^6,$$

$$C_3 = L_J J^8 + L_{JJK} J^6 J_z^2 + L_{JK} J^4 J_z^4 + L_{JKK} J^2 J_z^6 + L_K J_z^8,$$

$$b_0 = \frac{B - C}{2}; \qquad b_1 = -\delta_3 J^2 - \delta_K J_z^2,$$

$$b_2 = h_J J^4 + h_{JK} J^2 J_z^2 + h_K J_z^4$$

$$b_3 = l_J J^6 + l_{JK} J^4 J_z^2 + l_{KJ} J^2 J_z^4 + l_K J_z^4. \tag{1}$$

The divergence of this series beginning with certain rotational quantum numbers is illustrated in the first column of Table I. The numerical values of the diagonal matrix elements for $J = 20$, and $K = 20$ of the ground state of $H_2^{16}O$ are presented there. They were obtained by perturbation theory from the rotational constants given in Ref. (2), from the 0th order (J^2) to the 6th order (J^{14}), inclusive. The divergence of the series (1) is not something unusual for perturbation theory; e.g., for one of the simplest quantum systems, an anharmonic oscillator with the Hamiltonian $H = -d^2/dx^2 + x^2 + \beta x^4$, the perturbation series is divergent for all values of β, as shown in Ref. (3, 4). Table II is taken from Ref. (4) and illustrates not only the divergence of the perturbation series for the energy of the anharmonic oscillator, but the convergence of the sequence of the Padé approximants as well. The use of Padé approximants is a method for summation of the divergent series (5) widely used in various physical problems. In Ref. (4) the convergence of the Padé approximants of the perturbation series for the energy of the anharmonic oscillator is illustrated numerically, as well as proven analytically. The Padé approximants method is the simplest but not the only one; e.g., in Ref. (6) the method of the Borel approximation is used for the calculation of the anharmonic energy. The authors of this work (6) used numerical examples to show that the

TABLE I

The Calculated Values of the Energy Level $20_{20\,0}$ of $H_2^{16}O$

	1	2	3
J^2	11 390.26	11 390.26	11 390.26
J^4	6 935.37	8 187.87	8 481.26
J^6	13 772.41	9 632.72	9 440.73
J^8	− 399.06	9 220.62	9 235.51
J^{10}	24 239.92		
J^{12}	− 2 344.12		
J^{14}	10 190.64		

Estimation of the energy value is made from the diagonal matrix element with $J = 20$, $K = 20$:1, by the perturbation series; 2, by the one-dimensional Padé approximation; 3, by the Borel approx. All values of the energy levels are given in cm^{-1}.

convergence of the Borel sequence to the exact solution is even more rapid than that of the Padé approximants. It seems natural for us to use the methods mentioned above for the calculation of the energy levels of molecules, i.e., for the approximation of the Hamiltonian (1). The second and third columns of Table I were obtained as a result of the application of Padé and Borel formulas, respectively, for the rearrangement of the parameters of the initial series (1) [these are formulas (3) and (4) in the second part of the report]. It is easily seen from Table I that the perturbation series is divergent (column 1), its Pade approximant is convergent (column 2), and its Borel approximant is convergent more rapidly (column 3) to the experimental value of 9257 cm^{-1} for the $20_{20\,0}$ level of the ground state of $H_2{}^{16}O$. These results are completely analogous to the results mentioned above for the anharmonic oscillator energy calculation. The values of parameters used in all calculations of Table I are taken directly from Ref. (2), that is, without any fitting of the parameters of Eqs. (3) and (4) to the experimental values. The results of such a fitting are presented in Part III of this paper. But first we pass to some details of the Padé and Borel methods as applied to the Hamiltonian (1) approximation.

PART II

The Pade approximant of the function $f(x) = \sum_k \alpha_K x^k$ is the ratio of two polynomials $P_m(x)$ and $Q_n(x)$ satisfying the relation $f(x) - P_m(x)/Q_n(x) = O(x^{m+n+1})$, where m and n are the powers of P and Q, respectively. The Padé approximant can be expressed in terms of the initial function coefficients as follows

$$f[m/n] = \frac{P_m(\chi)}{Q_n(\chi)} = \frac{\begin{vmatrix} \alpha_{m-n+1} & \alpha_{m-n+2} & \cdots & \alpha_{m+1} \\ \alpha_{m-n+2} & \alpha_{m-n+3} & & \alpha_{m+2} \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ \sum_{j=n}^{m} \alpha_{j-n}\chi^j & \sum_{j=n-1}^{m} \alpha_{j-n+1}\chi^j & \cdots & \sum_{j=0}^{m} \alpha_j\chi^j \end{vmatrix}}{\begin{vmatrix} \alpha_{m-n+1} & \alpha_{m-n+2} & \cdots & \alpha_{m+1} \\ \alpha_{m-n+2} & \alpha_{m-n+3} & \cdots & \alpha_{m+2} \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ \chi^n & \chi^{n-1} & & 1 \end{vmatrix}} \qquad (2)$$

The theory of approximants is developed only for one-dimensional functions. In particular, this concerns the unambiguous expression of the approximants in terms of parameters of the initial function. The proof of the monotonic convergence of the approximant sequence to the exact solution for the series of a certain kind also exists only for one-dimensional functions. Thus, we must find a way to consider the Hamiltonian (1) as a one-dimensional function in order to apply this theory to it, i.e., to construct its one-dimensional approximation. In particular, this goal can

TABLE II

Sum of the Perturbation Series and its Padé Approximants for the Ground State Energy Calculation
of the Anharmonic Oscillator with the Hamiltonian $H = -d^2/dx^2 + x^2 + \beta x^4$.

N	PERTURBATION SERIES	PADÉ APPROXIMANTS
1	1.150000	
2	1.097500	1.111111
3	1.153750	
4	1.105372	1.117541
5	1.176999	
6	1.049024	1.118183
7	1.314970	
8	0.686006	1.118273
9	2.353090	
10	− 2.442698	1.118288
11	13.253968	
12	− 42.333586	1.118289
13	168.895730	
14	− 796.466406	1.118289
15	3005.179546	

Exact value of the energy $E(\beta) = 1.118289$; $\beta = 0.2$.

be achieved if Hamiltonian (1) is considered as a function of the smallness
parameter. Applying formulas (2) to the Hamiltonian (1), in this case, we obtain
formulas for both H_{diag} and H_{nondiag} from the first to the third orders (from J^4 to
J^8)

$$^P H^{(4)}_{\text{diag}} = \frac{C_0^2}{C_0 - C_1}; \qquad ^P H^{(6)}_{\text{diag}} = C_0 + \frac{C_1^2}{C_1 - C_2};$$

$$^P H^{(8)}_{\text{diag}} = C_0 + \frac{C_1(C_0 C_2 - C_1^2) - C_0(C_3 C_1 - C_2^2)}{C_0 C_2 - C_1^2 + C_2 C_1 - C_0 C_3 + C_1 C_3 - C_2^2};$$

$$^P H^{(4)}_{\text{nondiag}} = \frac{b_0^2}{b_0 - b_1}; \qquad ^P H^{(6)}_{\text{nondiag}} = b_0 + \frac{b_1^2}{b_1 - b_2};$$

$$^P H^{(8)}_{\text{nondiag}} = b_0 + \frac{b_1(b_0 b_2 - b_1^2) - b_0(b_3 b_1 - b_2^2)}{b_0 b_2 - b_1^2 + b_2 b_1 - b_0 b_3 + b_1 b_3 - b_2^2}. \qquad (3)$$

Thus, we have convergent expressions (see Table I) that are only a rearrangement
of the terms in the divergent series (1) by formulas (3). Here we want to emphasize
that the parameters of (3) are the usual Watson parameters.

The use of the Borel method (6) for the construction of a one-dimensional
approximation of (1) results in the following expressions:

$$U_0 = C_0/1! \qquad U_1 = C_1/2! \qquad U_2 = C_2/3! \qquad U_3 = C_3/4!$$

$$^B H^{(4)}_{\text{diag}} = \int_0^\infty e^{-\chi} \frac{U_0^2 \chi}{U_0 - U_1 \chi} d\chi,$$

$$^BH^{(6)}_{\text{diag}} = \int_0^\infty e^{-\chi} \chi \, \frac{U_1(U_0 + U_1\chi) - U_0U_2\chi}{U_1 - U_2\chi} \, d\chi,$$

$$^BH^{(8)}_{\text{diag}} = \int_0^\infty e^{-\chi} \, \frac{(U_0^2U_2 - U_1^2U_0)\chi + (2U_0U_1U_2 - U_0^2U_3 - U_1^3)\chi^2}{U_0U_2 - U_1^2 + (U_2U_1 - U_0U_3)\chi + (U_1U_3 - U_2^2)\chi^2} \, d\chi. \tag{4}$$

PART III

Using the method proposed, we carried out a fitting of the experimental data on the ground state of $H_2{}^{16}O$. In a model of 30 parameters up to J^{10} with the Padé method applied to the approximation of both diagonal and nondiagonal parts of Eq. (1), all available data on the $H_2{}^{16}O$ ground state, MW (7, 8), FIR (9), and the energy levels of (1) were fitted. As a result, we obtained a standard deviation

$$\sigma = \left[\sum_i^N \left(\frac{\nu^i_{\text{OBs}} - \nu^i_{\text{Cal}}}{\sigma_i} \right)^2 \bigg/ N - P \right]^{1/2}, \tag{5}$$

(where N is the number of lines and P is the number of model parameters) that is equal to 3 both for MW and FIR data, and the maximum difference between the calculated and experimental levels of (1) does not exceed 3 cm^{-1}. We do not present here the calculated energy of the levels and the values of parameters of this fitting because the use of the Borel method for approximation of the diagonal part enables one to obtain similar results with a model of 24 parameters up to J^8, due to a more rapid convergence of the Borel approximants (see Table I).

The following Hamiltonian was used in the final fitting

$$H = {}^BH^{(8)}_{\text{diag}} + \frac{1}{2} \, {}^PH^{(8)}_{\text{nondiag}}(J_x^2 - J_y^2) + \frac{1}{2}(J_x^2 - J_y^2){}^PH^{(8)}_{\text{nondiag}} \tag{6}$$

TABLE III

Rotational Constants of the $H_2{}^{16}O$ Molecule in the Ground State

A	835 838.592160	$h_J \times 10^2$	0.8332878806
B	435 348.769544	$h_{JK} \times 10$	-0.2010365094
C	278 139.834584	h_K	0.9371714642
Δ_J	37.6187302	$L_J \times 10^4$	-0.1573457432
Δ_{JK}	-173.3635582	$L_{JJK} \times 10^3$	0.1493319400
Δ_K	973.9394806	$L_{JK} \times 10^2$	-0.2374869033
δ_J	15.23720172	$L_{JKK} \times 10^2$	0.9593506036
δ_K	39.89372268	$L_K \times 10$	-0.2722414285
$H_J \times 10$	0.170739615	$l_J \times 10^5$	-0.6060448400
$H_{JK} \times 10$	-0.585801012	$l_{JK} \times 10^6$	0.7847884875
H_{KJ}	-0.531237765	$l_{KJ} \times 10^3$	0.3657600240
H_K	3.829370008	$l_K \times 10$	-0.1087736290

All values of constants are given in MHz.

TABLE IV

The Rotational Energy Levels of $H_2{}^{16}O$ in the Ground State Calculated from the Model of Eq. (4) with Rotational Constants from Table III (I, the assignment of levels; II, the energy of the levels in cm^{-1})

I			II	I			II	I			II
1	0	1	23.7944	7	5	3	1059.6446	10	8	3	2254.3514
1	1	1	37.1371	7	5	2	1059.8334	10	8	2	2254.3521
1	1	0	42.3718	7	6	2	1216.1939	10	9	2	2471.4059
2	0	2	70.0909	7	6	1	1216.1987	10	9	1	2471.4059
2	1	2	79.4964	7	7	1	1394.8188	10	10	1	2702.0266
2	1	1	95.1760	7	7	0	1394.8188	10	10	0	2702.0266
2	2	1	134.9017	8	0	8	744.0640	11	0	11	1327.1065
2	2	0	136.1640	8	1	8	744.1630	11	1	11	1327.1137
3	0	3	136.7618	8	1	7	882.8901	11	1	10	1524.8437
3	1	3	142.2785	8	2	7	885.5999	11	2	10	1525.1327
3	1	2	173.3660	8	2	6	982.9114	11	2	9	1690.6605
3	2	2	206.3015	8	3	6	1006.1147	11	3	9	1695.0670
3	2	1	212.1565	8	3	5	1050.1569	11	3	8	1813.2199
3	3	1	285.2195	8	4	5	1122.7053	11	4	8	1843.0221
3	3	0	285.4188	8	4	4	1131.7730	11	4	7	1899.0031
4	0	4	222.0530	8	5	4	1255.1599	11	5	7	1985.7797
4	1	4	224.8385	8	5	3	1255.9049	11	5	6	1998.9936
4	1	3	275.4974	8	6	3	1411.6123	11	6	6	2142.5681
4	2	3	300.3625	8	6	2	1411.6428	11	6	5	2144.0186
4	2	2	315.7797	8	7	2	1590.7105	11	7	5	2321.7805
4	3	2	382.5170	8	7	1	1590.7111	11	7	4	2321.8734
4	3	1	383.8426	8	8	1	1789.0667	11	8	4	2522.2958
4	4	1	488.1077	8	8	0	1789.0667	11	8	3	2522.2996
4	4	0	488.1341	9	0	9	920.1684	11	9	3	2740.5955
5	0	5	325.3482	9	1	9	920.2099	11	9	2	2740.5956
5	1	5	326.6257	9	1	8	1079.0781	11	10	2	2973.1305
5	1	4	399.4580	9	2	8	1080.3849	11	10	1	2973.1305
5	2	4	416.2090	9	2	7	1201.9208	11	11	1	3216.4352
5	2	3	446.5109	9	3	7	1216.2285	11	11	0	3216.4352
5	3	3	503.9680	9	3	6	1282.9171	12	0	12	1557.8352
5	3	2	508.8119	9	4	6	1340.8823	12	1	12	1557.8385
5	4	2	610.1144	9	4	5	1360.2340	12	1	11	1774.6114
5	4	1	610.3411	9	5	5	1474.9697	12	2	11	1774.7447
5	5	1	742.0721	9	5	4	1477.2872	12	2	10	1960.2027
5	5	0	742.0754	9	6	4	1631.2355	12	3	10	1962.5105
6	0	6	446.6969	9	6	3	1631.3723	12	3	9	2105.8661
6	1	6	447.2527	9	7	3	1810.6014	12	4	9	2124.9437
6	1	5	542.9063	9	7	2	1810.6060	12	4	8	2205.6450
6	2	5	552.9116	9	8	2	2009.8682	12	5	8	2275.3702
6	2	4	602.7738	9	8	1	2009.8683	12	5	7	2300.6857
6	3	4	648.9784	9	9	1	2225.5355	12	6	7	2433.7783
6	3	3	661.5486	9	9	0	2225.5355	12	6	6	2437.4842
6	4	3	756.7238	10	0	10	1114.5314	12	7	6	2612.7431
6	4	2	757.7792	10	1	10	1114.5486	12	7	5	2613.0490
6	5	2	888.5989	10	1	9	1293.0151	12	8	5	2813.4873
6	5	1	888.6328	10	2	9	1293.6328	12	8	4	2813.5039
6	6	1	1045.0570	10	2	8	1437.9670	12	9	4	3032.8191
6	6	0	1045.0574	10	3	8	1446.1246	12	9	3	3032.8197
7	0	7	586.2439	10	3	7	1538.1460	12	10	3	3267.1329
7	1	7	586.4796	10	4	7	1581.3321	12	10	2	3267.1329
7	1	6	704.2144	10	4	6	1616.4511	12	11	2	3512.9403
7	2	6	709.6083	10	5	6	1718.7084	12	11	1	3512.9403
7	2	5	782.4100	10	5	5	1724.6972	12	12	1	3766.7488
7	3	5	816.6938	10	6	5	1874.9499	12	12	0	3766.7488
7	3	4	842.3563	10	6	4	1875.4394	13	0	13	1806.6501
7	4	4	927.7413	10	7	4	2054.3428	13	1	13	1806.6519
7	4	3	931.2347	10	7	3	2054.3663	13	1	12	2042.3039

TABLE IV—*Continued*

I			II	I			II	I			II
13	2	12	2042.3645	15	3	13	2872.6232	16	16	0	6290.2309
13	2	11	2246.8863	15	3	12	3080.2113	17	0	17	2981.1648
13	3	11	2248.0748	15	4	12	3083.9298	17	1	17	2981.1640
13	3	10	2414.7231	15	4	11	3244.6183	17	1	16	3291.1113
13	4	10	2426.1998	15	5	11	3269.5752	17	2	16	3291.1158
13	4	9	2533.7877	15	5	10	3360.6002	17	2	15	3567.3305
13	5	9	2586.5251	15	6	10	3443.2119	17	3	15	3567.4108
13	5	8	2629.3308	15	6	9	3472.8965	17	3	14	3811.1278
13	6	8	2748.0953	15	7	9	3624.1894	17	4	14	3812.2423
13	6	7	2756.4173	15	7	8	3629.1131	17	4	13	4018.0218
13	7	7	2927.0162	15	8	8	3824.4018	17	5	13	4027.7087
13	7	6	2927.8852	15	8	7	3824.9048	17	5	12	4174.3364
13	8	6	3127.7177	15	9	7	4045.0965	17	6	12	4221.1623
13	8	5	3127.7747	15	9	6	4045.1331	17	6	11	4291.9380
13	9	5	3347.8077	15	10	6	4283.2509	17	7	11	4409.4266
13	9	4	3347.8106	15	10	5	4283.2529	17	7	10	4428.1864
13	10	4	3583.6920	15	11	5	4535.3856	17	8	10	4610.0680
13	10	3	3583.6921	15	11	4	4535.3857	17	8	9	4612.8470
13	11	3	3831.8569	15	12	4	4798.0960	17	9	9	4830.4717
13	11	2	3831.8569	15	12	3	4798.0960	17	9	8	4830.7550
13	12	2	4088.8350	15	13	3	5067.9567	17	10	8	5069.6341
13	12	1	4088.8350	15	13	2	5067.9567	17	10	7	5069.6561
13	13	1	4351.0580	15	14	2	5341.3867	17	11	7	5324.3793
13	13	0	4351.0580	15	14	1	5341.3867	17	11	6	5324.3807
14	0	14	2073.4764	15	15	1	5614.4866	17	12	6	5591.4880
14	1	14	2073.4773	15	15	0	5614.4866	17	12	5	5591.4880
14	1	13	2327.8730	16	0	16	2660.8262	17	13	5	5867.7385
14	2	13	2327.9015	16	1	16	2660.8269	17	13	4	5867.7385
14	2	12	2550.9016	16	1	15	2952.3610	17	14	4	6149.7935
14	3	12	2551.5042	16	2	15	2952.3703	17	14	3	6149.7935
14	3	11	2739.4347	16	2	14	3211.1479	17	15	3	6434.1017
14	4	11	2746.0517	16	3	14	3211.2980	17	15	2	6434.1017
14	4	10	2880.8377	16	3	13	3437.3697	17	16	2	6716.7604
14	5	10	2918.2470	16	4	13	3439.4220	17	16	1	6716.7604
14	5	9	2983.3897	16	4	12	3623.8108	17	17	1	6993.2077
14	6	9	3084.8461	16	5	12	3639.6414	17	17	0	6993.2077
14	6	8	3101.4559	16	5	11	3758.4154				
14	7	8	3264.3040	16	6	11	3822.2933	18	0	18	3319.1418
14	7	7	3266.4870	16	6	10	3870.2180	18	1	18	3319.1411
14	8	7	3464.7722	16	7	10	4006.1194	18	1	17	3647.4041
14	8	6	3464.9562	16	7	9	4016.1869	18	2	17	3647.4038
14	9	6	3685.3123	16	8	9	4206.2968	18	2	16	3940.8000
14	9	5	3685.3234	16	8	8	4207.5348	18	3	16	3940.8477
14	10	5	3922.4922	16	9	8	4426.9125	18	3	15	4201.5833
14	10	4	3922.4927	16	9	7	4427.0199	18	4	15	4202.1850
14	11	4	4172.7900	16	10	7	4665.7141	18	4	14	4427.4139
14	11	3	4172.7900	16	10	6	4665.7211	18	5	14	4433.1975
14	12	3	4432.7643	16	11	6	4919.3365	18	5	13	4606.2744
14	12	2	4432.7643	16	11	5	4919.3365	18	6	13	4638.9070
14	13	2	4698.9168	16	12	5	5184.4450	18	6	12	4735.9034
14	13	1	4698.9168	16	12	4	5184.4450	18	7	12	4833.3588
14	14	1	4967.5467	16	13	4	5457.6999	18	7	11	4865.3201
14	14	0	4967.5467	16	13	3	5457.6999	18	8	11	5035.2478
15	0	15	2358.2318	16	14	3	5735.6366	18	8	10	5040.9882
15	1	15	2358.2319	16	14	2	5735.6366	18	9	10	5255.5430
15	1	14	2631.2518	16	15	2	6014.5399	18	9	9	5256.1118
15	2	14	2631.2613	16	15	1	6014.5399	18	10	9	5494.7341
15	2	13	2872.3230	16	16	1	6290.2309	18	10	8	5494.7954

TABLE IV—*Continued*

I			II	I			II	I			II
18	11	8	5750.2746	19	8	11	5492.2755	20	5	16	5294.8479
18	11	7	5750.2790	19	9	11	5701.3978	20	5	15	5513.7022
18	12	7	6018.9615	19	9	10	5702.9121	20	6	15	5527.7769
18	12	6	6018.9617	19	10	10	5940.6788	20	6	14	5680.9559
18	13	6	6297.7419	19	10	9	5940.8350	20	7	14	5739.7610
18	13	5	6297.7419	19	11	9	6196.7680	20	7	13	5812.2444
18	14	5	6583.4385	19	11	8	6196.7808	20	8	13	5947.6435
18	14	4	6583.4385	19	12	8	6466.6431	20	8	12	5967.0912
18	15	4	6872.6637	19	12	7	6466.6439	20	9	12	6167.9623
18	15	3	6872.6637	19	13	7	6747.4548	20	9	11	6171.0920
18	16	3	7161.7392	19	13	6	6747.4548	20	10	11	6407.0800
18	16	2	7161.7392	19	14	6	7036.2431	20	10	10	6407.4471
18	17	2	7446.5181	19	14	5	7036.2431	20	11	10	6663.5470
18	17	1	7446.5181	19	15	5	7329.8116	20	11	9	6663.5813
18	18	1	7721.9164	19	15	4	7329.8116	20	12	9	6934.3117
18	18	0	7721.9164	19	16	4	7624.6847	20	12	8	6934.3143
19	0	19	3674.6463	19	16	3	7624.6847	20	13	8	7216.6801
19	1	19	3674.6462	19	17	3	7917.0214	20	13	7	7216.6802
19	1	18	4021.1330	19	17	2	7917.0214	20	14	7	7507.9686
19	2	18	4021.1290	19	18	2	8202.3673	20	14	6	7507.9686
19	2	17	4331.4678	19	18	1	8202.3673	20	15	6	7805.2317
19	3	17	4331.4960	19	19	1	8474.9253	20	15	5	7805.2317
19	3	16	4608.7509	19	19	0	8474.9253	20	16	5	8105.2091
19	4	16	4609.0843	20	0	20	4047.5595	20	16	4	8105.2091
19	4	15	4852.2877	20	1	20	4047.5600	20	17	4	8404.3106
19	5	15	4855.6806	20	1	19	4412.1847	20	17	3	8404.3106
19	5	14	5052.8986	20	2	19	4412.1791	20	18	3	8698.5029
19	6	14	5074.6851	20	2	18	4739.2312	20	18	2	8698.5029
19	6	13	5199.6954	20	3	18	4739.2431	20	19	2	8982.9497
19	7	13	5277.0938	20	3	17	5032.5952	20	19	1	8982.9497
19	7	12	5327.1129	20	4	17	5032.7908	20	20	1	9250.8721
19	8	12	5481.3050	20	4	16	5292.8749	20	20	0	9250.8721

where $^{B}H_{diag}^{(8)}$ and $^{P}H_{nondiag}^{(8)}$ are the same as in Eqs. (4) and (3). The energy levels up to $J = 20$ and $K = 20$ from Ref. (*1*) were used in the fitting. Only $5L$ parameters were fit, while all other parameters were fixed to the values obtained by the previous Padé fitting.

In Table III the rotational constants obtained for the Hamiltonian (6) are presented and in Table IV the calculated values of the energy levels up to $J = 20$ and $K = 20$ are given. It is easily seen from a comparison of the data in Table IV and the experimental levels of Ref. (*1*) that the maximum difference between the calculated and experimental levels does not exceed 8 cm^{-1} in the model of 24 parameters up to J^8. This difference decreases with decreasing in J and K.

CONCLUSIONS

It is possible to obtain a still more rapid convergence of the Borel approximant sequences by some modification of this method. In particular, the preliminary calculations show that the use of this modification results in a decrease in the maximum difference between the observed and the calculated energy values to 1.5

cm^{-1} without additional fitting and expansion of the model. In the future, we are planning to carry out a joint fitting of MW and FIR data and the data of Ref. (*1*) using this modification in the model of 24 parameters, which we hope will reproduce the observed data to within the experimental errors.

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