USE OF GENERATING FUNCTIONS IN CALCULATIONS OF ROVIBRATIONAL ENERGIES OF THE CH_2 RADICAL

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This paper presents a discussion of qualitative studies of the rotational energy of nonrigid molecules of H_2X *type on the quantum number K characterizing a projection of the angular momentum operator onto the molecular linearization axis Z. The frequencies of rotational and rovibrational transitions are processed for the* CH_2 *molecule using the generating functions for an effective rotational Hamiltonian. Rotational energies of the vibrational states* (000) *and* (010) *are reconstructed.*

INTRODUCTION

The methyl radical CH_2 is one of the simplest free radicals playing an important role in molecular spectroscopy and chemistry.[1–6] The presence of this molecule in the upper layers of the atmosphere, comet tails, and interstellar space may also be mentioned. From a spectroscopic point of view, CH_2 attracts particular interest because it is one of the simplest neutral molecules with a triplet ground electronic state. Moreover, the CH_2 molecule, as well as other light molecules (H_2O, NH_2, ...), possess bending vibration of large amplitude. However, in contrast to other such molecules, the effects of nonrigidity, due to this vibration, are much stronger in CH_2 and caused by the fact that an equilibrium configuration of this molecule is close to the linear one. According to estimates from Ref. 6 the energy barrier h between the actual and a linear configuration of the molecule is about 1900 cm^{-1}. For the H_2O molecule, $h \simeq 10055–10900$ cm^{-1}, (see Ref. 7).

One of the consequences of the nonrigidity effects in CH_2 is the divergence of the effective rotational Hamiltonian (in Watson form) used for processing the experimental results

$$\mathbf{H}_W = \sum_{ij} a_{ij} \mathbf{N}^{2i} \mathbf{N}_z^{2j} + \sum_{ij} b_{ij} \mathbf{N}^{2i} \{\mathbf{N}_z^{2j}, \mathbf{N}_x^2 - \mathbf{N}_y^2\} , \quad (1)$$

where $\mathbf{N}_x$, $\mathbf{N}_y$, and $\mathbf{N}_z$ are components of the operator of angular momentum $\mathbf{N}$ with respect to the molecular system of axes in the I_r representation. A large number of centrifugal distortion constants in $\mathbf{H}_W$ is indicative of its divergence. Thus, in Ref. 1 eleven constants for processing of fourteen rotational transitions were used. In Ref. 5 some parameters of series (1) were fixed by taking for their values those obtained by processing the energy levels previously calculated from the molecular force field.

In the literature (see, e.g., Refs. 3 and 6) there are some methods of correct account for rovibrational interaction which allow one to reconstruct the molecular energy levels from the force field. However, the precision of these methods in reconstructing the experimental results is lower than that of the method, where the Hamiltonian $\mathbf{H}_W$ is used, in spite of its divergence.

This paper deals with the following problems. First, the dependence of rotational energy of a triatomic H_2X molecule on the rotational quantum number K is analyzed qualitatively. Second, the generating functions are constructed for the rotational Hamiltonian $\mathbf{H}_r$ of the CH_2 molecule which are then used for processing of frequencies of the rotational and rovibrational transitions, and third, the rotational energy levels of the ground and (010) vibrational states of this molecule are calculated using the parameters of the rotational Hamiltonian $\mathbf{H}_r$ obtained from the processing of frequencies.

1. QUALITATIVE ANALYSIS OF THE K–DEPENDENCE OF THE ROTATIONAL ENERGY OF H_2X MOLECULES

In the rotational Hamiltonian $\mathbf{H}_W$ the subsequences containing powers of the operator J_Z^2 (Z is the linearization axis of the molecule) are most long. The inverse tensor of inertia $A(\rho)$ undergoes a strong change with respect to this axis during a large amplitude vibration. The coordinate $\rho = \pi - \gamma$ describes a vibration of a large amplitude where γ is the HXH angle in the reference configuration of the molecule.[7] A diagonal part of the Hamiltonian (1) in the basis of wave functions $|J, K>$ takes the form (although in the general case $J = N + S$, here the case of $S = 0$ is considered)

$$h^J(K) = \sum_i a_i(J) K^{2i} = < J, K \,|\mathbf{H}_W^{\rm diag}|\, J, K > , \quad (2)$$

with the J–dependent parameters a_i:

$$a_i(J) = a_{0i} + a_{1i} J(J + 1) + a_{2i} [J(J + 1)]^2 + \dots . \quad (3)$$

Subsequences of the type (3) converge sufficiently rapidly, therefore in the subsequent discussion the convergence of series (2) with respect to the quantum number K is considered, J being assumed to be fixed (the index J is omitted below). The function $h^J(K)$ (for which the coefficients of Taylor expansion coincide with the parameters of Eq. (3)) can be reconstructed, in the first approximation, based on numerical integration of the Schrödinger equation

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$$\left\{ -\mu \frac{\partial^2}{\partial\rho^2} + V_0(\rho) + A(\rho)\, K^2 \right\} \psi = h(K)\, \psi \qquad (4)$$

with the potential function $V_0(\rho)$ and function $A(\rho)$ being preset.

For triatomic molecules of the H_2X type

$$A(\rho) = a/\sin^2(\rho/2)\ ; \quad a = h/8\pi^2 c(1 + \delta)/(2m_H\, r_0^2)\ ;$$

$$\delta = 2m_H/m_X\ . \qquad (5)$$

where m_H and m_X are the masses of atoms H and X, respectively, and r_0 is the distance between these atoms in the reference configuration of the molecule. In this study we are interested in a possible analytical form of the function $h(K)$ therefore let us pass from Eq. (4) to estimation of the molecular energy based on the following relation[8]

$$h(K) = N/2L^2\mu + V_0(L) + A(L)\, K^2\ . \qquad (6)$$

In Eq. (6) $N = (n + 1/2)^2$, n is the vibrational quantum number, and L is the specific length of the region of ρ variation which is determined from the condition $\partial h/\partial L = 0$. For a harmonic oscillator $V_0(\rho) = \omega^2/2\mu(\rho - \rho_e)^2$ and Eq. (6) in combination with the condition $\partial h/\partial L = 0$ are written in the form (ρ_e is the equilibrium value of the angle ρ)

$$h(K) = N/2L^2\mu + \omega^2 L^2/2\mu + aK^2/\sin^2((L + \rho_e)/2)\ , \qquad (7)$$

$$\partial h/\partial L = 0 = -N/L^3\mu + \omega^2 L/\mu - \frac{aK^2 \sin(L + \rho_e)}{2\sin^4((L + \rho_e)/2)}\ . \qquad (7a)$$

The n dependence, as in Ref. 8, is chosen so that at $K = 0$ we obtain the exact solution for the harmonic oscillator $h(K = 0) = \omega(n + 1/2)$.

A complicated behavior of the inverse tensor of inertia $A(\rho)$ does not make it possible to find the exact solution for L from Eq. (7a) in the general form and to estimate $h(K)$. Consider three groups of molecules with the specific value ρ_e.

A. A group of quasilinear molecules with ρ_e | 0. By expanding in Eqs. (7) and (7a) the last terms into a series over the value $\rho_e/L < 1$ and taking into account only the first terms of these expansions (in zero approximation), we have

$$L_0 = (N + 8\, aK^2/\mu)\mu^2/\omega^2\ ,$$

$$h_0(K) = h(K, L_0) = \omega \sqrt{(n + 1/2)^2 + 8\, aK^2/\mu}\ . \qquad (8)$$

For triatomic molecules of the H_2X type, $\mu = B_q(\rho_e) \simeq 4a$, where a g 10 cm^{-1} at $r_0 \simeq 1$ Å. Depicted in Fig. 1 are the dependences $h_0(K)$ calculated by Eq. (8) (with respect to the level $h(K = 0)$) for the above values of a and μ and $\omega = 250$ cm^{-1} and 1000 cm^{-1} and $\rho_e = 0.05$ rad ($n = 0$). Dashed lines in the figure denote the dependence $h(K)$ obtained from numerical solution of Eq. (7) for the same values of ω and ρ_e. It can be well seen that the functions $h_0(K)$ give the linear dependence on K even at small K values since the relation $8\, aK^2/\mu \gg N^2$ is valid for them what reduces Eq. (8) to the relation $h_0(K) \simeq \theta|K|$, where θ is a constant. The circles in Fig. 1 denote the intervals where the functions $h(K)$ give approximately linear dependence on K. Thus the functions $h(K)$ have the form of straight lines "joined" at certain values of the quantum number K. To describe this function using a power series of the type (2) one should have approximately as many variable parameters a_i as the number of the values of the function $h(K)$. If the energy level with $K = 0$ is taken as the reference energy level then instead of $h_0(K)$ it is convenient to introduce the function

$$G(K) = \frac{\sqrt{1 + \alpha K^2} - 1}{2\alpha} \qquad (9)$$

with the J—dependent parameter α

$$\alpha = \alpha_0 + \alpha_1 J(J + 1) + \alpha_2[J(J + 1)]^2 + \dots\ .$$

Function (9) was first introduced in Refs. 9 and 10 for the water molecule and was generalized in Refs. 11 and 12. The function (9) differs from those considered in Refs. 9–12 by the fact that the parameter $\alpha_0 > 1$, and this is the specific feature of quasilinear molecules.

The functions $h(K)$ obtained from Eq. (7) (dashed curves in Fig. 1) can be described by the analytical relation[9–12]

$$h(K) = \gamma_1 G + \gamma_2 G^2 + \gamma_3 G^3 + \dots\ . \qquad (10)$$

In particular, for $\omega = 250$ cm^{-1} (the lower dashed curve in Fig. 1) to describe the first ten values accurate to $\simeq 1$ cm^{-1} it is sufficient to take three variable parameters γ_i in Eq. (10). In this case $\alpha = 4.6$. To obtain the same accuracy with polynomial representation (2), ten parameters a_i are needed, since nine parameters from Eq. (2) give maximum divergence about 20 cm^{-1} in reconstructing this curve.

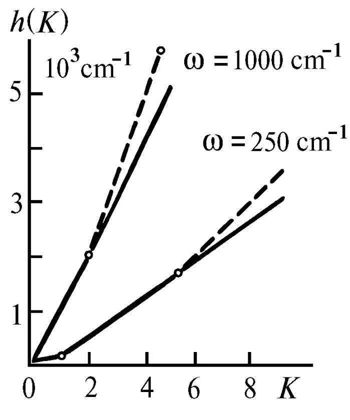

FIG. 1. Calculated by Eq. (8) (solid lines) and Eq. (7) (dashed lines) dependences of rotational energy of a quasilinear triatomic molecule of the type H_2X *(with* $\rho_e = 0.05$ rad*) on the quantum number K (for a hypothetical level J = 0).*

B. Molecules with ρ_e | π. By substituting $\pi = \rho_e + \gamma_e$ and expanding, as in the previous case, the last component of Eq. (8) over the value $\gamma_e/L < 1$, we obtain in zero approximation

$$h_0(K) = h_0(K, L_0) = aK^2 + \omega(n + 1/2)\sqrt{1 + a\mu K^2/2\omega^2}. \quad (11)$$

In relation (11) the first term describes rotational energy of a rigid–top

$$E_{rt} = aK^2 ,$$

and the second term accounts for the rovibrational interaction in the molecule and can be considered as a correction to E_{rt}. For a wide range of quantum numbers, the square root in Eq. (11) can be expanded into a series of type (2), and for the ratio of constants a_i in this series one can obtain the estimate

$$|a_{i+1}/a_i| = a\mu/4\omega^2 , \quad i > 1 .$$

The radius of convergence R_c of such a series can be determined from the relation

$$R_c = \omega\sqrt{2/a\mu} .$$

For the molecules of the H_2X type at the frequencies ω of the order of 1000 cm^{-1} $R_c \simeq 80$ and the ratio $|a_{i+1}/a_i| \simeq 10^{-4}$. It is evident that for such molecules the terms describing the rovibrational interaction can be related to perturbation, the series of the perturbation theory being convergent.

C. Molecules for which $\rho_e \simeq L$. This group of molecules is obviously intermediate between the above considered. Such nonrigid molecules as H_2O, NH_2, etc. are also attributed to it. It is not possible to obtain analytical solution for L from Eq. (7) in any reasonable approximation. These solutions can be obtained for different values of the parameters ρ_e, ω, a, and μ. Figure 2 depicts the energies $h(K)$ calculated by Eq. (7) for different values of ρ_e at the frequency ω = 1500 cm^{-1}.

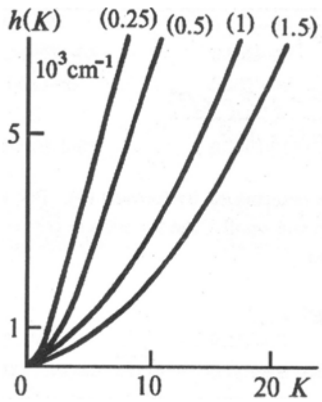

FIG. 2. Calculated by Eq. (7) dependences of rotational energy of nonrigid triatomic molecules of the H_2X *type on the quantum number K (for a hypothetical level J = 0 and* ω = 1500 cm^{-1}*). The value of an equilibrium angle* ρ_e *is given in parentheses.*

2. GENERATING FUNCTIONS FOR THE EFFECTIVE ROTATIONAL HAMILTONIAN H_r OF A MOLECULE OF THE H_2X TYPE

The effective rotational Hamiltonian $\mathbf{H}_r$ of the asymmetric top molecule can be written in the general form[10] as follows:

$$\mathbf{H}_r = F(\mathbf{J}^2, \mathbf{J}_z^2) + \{\chi(\mathbf{J}^2, \mathbf{J}_z^2), \mathbf{J}_{xy}^2\} . \quad (12)$$

The functions F and χ are called generating functions for diagonal and off–diagonal (in the basis of rotational wave functions $|J, K>$) parts of the Hamiltonian $\mathbf{H}_r$. The expansion of these functions into the Taylor series results in polynomial representation (1) for $\mathbf{H}_r$.

Let us turn back to Eq. (4) in which only the coordinate ρ is the dynamic variable. The quantum number K enters into Eq. (4) as a parameter. The function $h(K)$ can be considered as zero approach F_0 to the function $F(K) = <J, K|F|J, K>$. Equation (4) implies analytical solution for some forms of the potential function $V_0(\rho)$ and $K = 0$. Simulation of the function $A(\rho)$ by some function $\tilde{A}(\rho)$ with the same qualitative behavior, within the interval of ρ variation, as the function $A(\rho)$ can provide the solution for $h(K)$ at $K \neq 0$ as well, see Refs. 13 and 14. The main contribution of F_0 to the function F is determined from the relation

$$F_0 = h(K) - h(K = 0) \quad (13)$$

describing the rotational structure of this vibrational state. In particular, for $V_0(\rho) = \sum_{k=0}^{2} c_k\, th^k\alpha(\rho - \rho_e)$ and $\tilde{A}(\rho) = \sum_{k=0}^{2} \tilde{a}_k \times$ $\times\, th^k\alpha(\rho - \rho_e)$ the solution F_0 can be written in the form (if in the formula for h from Ref. 13 we make a substitution $K^2 = \gamma_1 G + \gamma_2 G^2$)

$$F_0 = \frac{g_1 G + g_2 G^2 + g_3 G^3 + g_4 G^4}{1 + \beta_1 G + \beta_2 G^2} . \quad (14)$$

In Eq. (14) G is determined by formula (9). For small values of the parameter α and small K the function G can be expanded into the Taylor series

$$G(K) = K^2 + \chi K^4 + \ldots . \quad (15)$$

The convergence radius $R_c = \sqrt{1/\alpha}$ of the expansion (15) is determined from condition $\alpha K^2 = 1$, (see Refs. 9 and 10). Following the qualitative consideration made in Sec. 1 it is possible to assume that for a quasilinear molecule of the CH_2 type the parameter α, at least for some vibrational states, proves to be sufficiently large and in function (14) it is necessary to make the substitution $G \to \chi|K|$. The generating function F_0 takes the form

$$\tilde{F}_0 = \frac{\tilde{g}_1|K| + \tilde{g}_2 K^2 + \ldots}{1 + \tilde{\beta}_1|K| + \ldots} . \quad (16)$$

3. PROCESSING OF THE EXPERIMENTAL DATA ON THE RADICAL CH_2

We have used in our study the functions (14) and (16) for processing frequencies of rotational and rovibrational transitions of the radical CH_2 given in Ref. 1. In the first case the function

$$\chi = \sum_{ij} b^*_{ij}\, \mathbf{N}^{2i} \{\mathbf{G}^j, \mathbf{N}_x^2 - \mathbf{N}_y^2\} \quad (17)$$

was used as an off–diagonal part of the Hamiltonian $\mathbf{H}_r$ and in the second case it was the function

$$\chi_W = \sum_{ij} b_{ij}\, \mathbf{N}^{2i} \{\mathbf{N}_z^{2j}, \mathbf{N}_x^2 - \mathbf{N}_y^2\} , \qquad (18)$$

coinciding with the off–diagonal part of the expansion (1). Let the Hamiltonian composed of functions (14) and (17) be called $\mathbf{H}_G$ and that composed of functions (10) and (18) $\mathbf{H}_{LIN}$. In both cases the function $g_0(N)$ determining the value of the molecular energy with $K = 0$ is taken as the series

$$g_0(N) = g_{00} + g_{10} N(N + 1) + g_{20}[N(N + 1)]^2 + \dots .$$

Nineteen frequencies of rotational transitions with $N \le 7$ and $N_a \le 4$ are known for the ground state.[6] The quality of processing of the experimental data is characterized by the value

$$\Sigma = \sum_i (\nu_i^{obs} - \nu_i^{calc})^2 .$$

Table I lists the values of Σ obtained by processing these frequencies using different representations of the rotational Hamiltonian $\mathbf{H}_r$.

At the next step the frequencies of rotational transitions were processed in combination with frequencies of the rovibrational transitions of the band ν_2 (61 frequencies with $N \le 10$ and $N_a \le 1$, (see Ref. 6)). The combined processing yields $\Sigma \simeq 10^{-4}$ cm^{-2} for the models $\mathbf{H}_G$ and $\mathbf{H}_{LIN}$. The obtained parameters of the Hamiltonians are given in Table II.

As can be seen from the table, the value of the parameter α_0 in the G–function of the Hamiltonian $\mathbf{H}_G$ is about 0.3 for the ground state and $\alpha_0 \simeq 2.2$ for the state (010). Therefore the substitution $G \to \chi|K|$ transforming Eq. (14) to (16) is justified. For both these states the value $\alpha_0 K^2 > 1$ even for $K = 2$. The convergence radius R_c of power expansion of the Hamiltonian $\mathbf{H}_r$ can be estimated based on the value of the parameter α_0. For the ground vibrational state, $R_c \simeq 2$ and for the state (010) $R_c < 1$.

TABLE I. Comparison of the quality of processing Σ (in cm^{-2}*) of the frequencies of rotational transitions of the radical* CH_2 *made with different representations of* $\mathbf{H}_r$ *(L is the number of the used parameters).*

Form of $\mathbf{H}_r$	L	Σ, cm^{-2}
$\mathbf{H}_W$	8	190.0
$\mathbf{H}_G$	8	53.0
$\mathbf{H}_{LIN}$	8	0.2*
$\mathbf{H}_W$	15	2.0E–4
$\mathbf{H}_G$	15	4.0E–8
$\mathbf{H}_{LIN}$	15	3.0E–7

* For the function $\tilde{F}_0 = \tilde{g}_2 K/(1 + \beta_1|K|)$.

TABLE II. Parameters of the Hamiltonians $\mathbf{H}_G$ *and* $\mathbf{H}_{LIN}$ *obtained from solution of the inverse spectroscopic problem for the* CH_2 *molecule*.*

Parameter	Hamiltonian $\mathbf{H}_{LIN}$		Hamiltonian $\mathbf{H}_G$	
State (000)				
α_0	–	–	0.2941188	0.17E–03
α_1	–	–	0.424887E–03	0.10E–04
α_2	–	–	0.9548E–06	0.14E–06
g_{10}	7.81711	0.11E–03	7.81725	0.75E–04
g_{20}	–0.352374E–03	0.34E–05	–0.367706E–03	0.15E–05
g_{30}	–0.37858E–06	0.26E–07	–	–
g_{01}	0.662592	0.31E–02	66.349656	0.12E–02
g_{11}	0.62055E–02	0.13E–03	0.2224565E–01	0.94E–04
g_{21}	–0.26517E–04	0.32E–05	–	–
g_{02}	69.549475	0.45E–02	–	–
g_{12}	0.164757E–01	0.15E–03	0.72139E–02	0.34E–03
g_{22}	0.8765E–05	0.40E–05	0.17027E–04	0.25E–05
β_{01}	0.110125	0.27E–04	–0.197639E–01	0.26E–04
β_{11}	0.32495E–04	0.14E–05	0.6178E–04	0.42E–05
u_{00}	0.31495	0.12E–02	0.356777	0.39E–02
u_{10}	–	–	–0.9668E–04	0.66E–06
u_{01}	–0.166589E–01	0.14E–02	–0.68597E–01	0.49E–02
u_{11}	–0.92383E–04	0.66E–06	–	–
u_{02}	0.5599E–03	0.19E–03	0.7144E–02	0.75E–03

TABLE II (continued)

State (010)				
α_0	–	–	2.1707495	0.44E–03
α_1	–	–	0.673945E–02	0.38E–04
α_2	–	–	–0.13517E–03	0.11E–05
g_{00}	963.0973	0.11E–02	963.10127	0.11E–02
g_{10}	7.7283018	0.14E–03	7.727231	0.14E–03
g_{20}	–0.566482E–03	0.43E–05	–0.515128E–03	0.41E–05
g_{30}	0.9816E–07	0.27E–07	–0.35019E–06	0.26E–07
g_{01}	62.468	0.12E+01	214.065445	0.95E–02
g_{11}	0.50679	0.12E–01	0.2346553	0.75E–03
g_{21}	–	–	–0.109566E–02	0.15E–04
g_{02}	139.6274	0.28E+01	–	–
g_{12}	–0.98633	0.27E–01	–	–
β_{01}	0.312684	0.11E–01	–	–
β_{11}	–0.37323E–02	0.10E–03	–	–
u_{00}	0.70642	0.58E–02	0.94491	0.26E–02
u_{10}	0.8438E–03	0.15E–03	0.10199E–03	0.16E–04
u_{01}	–0.418743	0.63E–02	–0.872448	0.35E–02
u_{11}	–0.1021E–02	0.17E–03	–0.87734E–03	0.30E–04
u_{21}	–	–	0.12999E–04	0.18E–06
u_{02}	0.296466E–01	0.59E–03	–	–
u_{12}	0.8716E–04	0.17E–04	–	–

* The parameters u_{ij} have a sense of the parameters b^*_{ij} (from Eq. (17)) of the Hamiltonian $\mathbf{H}_G$ and b_{ij} (from Eq. (18)) of the Hamiltonian $\mathbf{H}_{\rm LIN}$. In the third and fourth columns there are standard deviations of the parameters.

4. CALCULATION OF ENERGY LEVELS

Rotational energies of the ground vibrational state and of the state (010) were calculated using the parameters listed in Table II. The rotational energy levels are given in Table III. Represented here, for comparison, are the energy levels obtained using the variational methods.[6] It is clear that the model of Hamiltonian $\mathbf{H}_{\rm LIN}$ gives the energy levels close to those obtained in Ref. 6. This means that the analytical solution resulting in generating function (16) is close to the solution from Ref. 6. The energy levels reveal a nearly linear dependence on the quantum number K ($\equiv N_a$) which coincides with the aforementioned qualitative consideration of $h(K)$.

TABLE III. Vibrational–rotational energy levels of the CH_2 *molecule calculated using different methods.*

N	N_a	N_c	(0, 0, 0)			(0, 1, 0)		
			$\mathbf{H}_G$	$\mathbf{H}_{\rm LIN}$	Ref. 6	$\mathbf{H}_G$	$\mathbf{H}_{\rm LIN}$	Ref. 6
0	0	0				963.10	963.08	963.07
1	0	1	15.63	15.63	15.63	978.55	978.55	978.52
	1	1	78.32	78.31	78.33	1132.02	1132.02	1131.93
	1	0	79.52	79.51	79.52	1133.29	1133.28	1133.20
2	0	2	46.87	46.87	46.86	1009.45	1009.44	1009.42
	1	2	108.46	108.46	108.46	1161.94	1161.94	1161.88
	1	1	112.04	112.04	112.03	1165.75	1165.75	1165.66
	2	1	276.27	276.27	276.23	1426.29	1430.72	1430.82
	2	0	276.29	276.29	276.24	1426.29	1430.72	1430.82
3	0	3	93.67	93.67	93.64	1055.75	1055.75	1055.72
	1	3	153.64	153.64	153.64	1206.81	1206.81	1206.78
	1	2	160.79	160.78	160.77	1214.40	1214.40	1214.33
	2	2	323.45	323.44	323.41	1473.44	1477.87	1477.99
	2	1	323.53	323.53	323.49	1473.44	1477.87	1478.00
	3	1	562.42	566.85	566.97	1753.39	1807.42	1812.44
	3	0	562.42	566.85	566.97	1753.39	1807.42	1812.44
4	0	4	155.95	155.95	155.90	1117.42	1117.42	1117.40
	1	4	213.83	213.83	213.83	1266.61	1266.60	1266.61
	1	3	225.71	225.72	225.69	1279.22	1279.22	1279.17
	2	3	386.29	386.29	386.27	1536.24	1540.67	1540.84
	2	2	386.54	386.54	386.52	1536.26	1540.69	1540.88

TABLE III. (continued)

	3	2	625.62	630.05	630.20	1818.06	1874.07	1875.73
	3	1	625.62	630.05	630.20	1818.07	1874.06	1875.73
	4	1	928.75	933.16	933.12	2104.26	2248.98	2275.75
	4	0	928.75	933.16	933.12	2104.25	2248.98	2257.75
5	0	5	233.61	233.62	233.55	1194.41	1194.40	1194.38
	1	5	289.00	289.00	289.00	1341.29	1341.29	1341.35
	1	4	306.76	306.76	306.73	1360.17	1360.17	1360.14
	2	4	464.77	464.77	464.76	1614.70	1619.12	1619.34
	2	3	465.34	465.34	465.34	1614.73	1619.16	1619.43
	3	3	704.56	708.98	709.19	1898.43	1953.58	1954.78
	3	2	704.56	708.99	709.19	1898.45	1953.58	1954.78
	4	2	1008.06	1012.48	1012.50	2191.45	2343.56	2337.27
	4	1	1008.06	1012.48	1012.50	2191.45	2343.56	2337.27
	5	1	1379.90	1362.72	1361.96	–	–	2755.38
	5	0	1379.90	1362.72	1361.96	–	–	2755.38
6	0	6	326.54	326.54	326.48	1286.64	1286.63	1286.62
	1	6	379.09	379.09	379.10	1430.87	1430.84	1430.96
	1	5	403.86	403.86	403.83	1457.17	1457.17	1457.18
	2	5	558.82	558.82	558.84	1708.80	1713.16	1713.45
	2	4	559.95	559.94	559.99	1708.87	1713.21	1713.62
	3	4	799.21	803.63	803.91	1994.44	2043.47	2049.53
	3	3	799.22	803.64	803.92	1994.52	2043.47	2049.55
	4	3	1103.13	1107.56	1107.69	2294.96	2403.42	2432.59
	4	2	1103.13	1107.56	1107.69	2294.60	2403.42	2432.59
	5	2	1475.12	1458.27	1457.63	–	–	2851.21
	5	1	1475.12	1458.27	1457.63	–	–	2851.21
	6	1	1926.62	1846.32	1844.24	–	–	3297.57
	6	0	1926.62	1846.32	1844.24	–	–	3297.57

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