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THEORETICAL HERMAN-WALLIS COEFFICIENTS FOR C_0^7 AND D_0^7 AND THE DIPOLE-MOMENT FUNCTION OF HCl

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Abstract—Theoretical expressions for the Herman–Wallis coefficients C_0^7 and D_0^7 and a correction term of order $2B_e/\omega_e$ times the leading term for C_0^6, have been derived in terms of the Dunham potential-energy parameters and series dipole-moment expansion coefficients by the method of computer algebra. After reviewing previous work on the extraction of the dipole-moment function for HCl from experimental data, the present results are applied to a determination of the series representation up to seventh order in the reduced displacement from the equilibrium internuclear separation. Coefficients for an alternate representation in terms of a Padé approximant are also obtained; this model dipole-moment function should enable one to estimate more accurately the higher overtone and highly excited hot-band intensities since it circumvents the divergence difficulties of the series expansion and has the correct asymptotic behavior at both small and large internuclear separations.

1. INTRODUCTION

In recent years, there has been much progress in both the experimental measurements and the theory of intensities for vibration-rotational lines of diatomic molecules.[1] The molecule for which accurate intensities have been measured for transitions to the highest vibrational state from the ground state is hydrogen chloride; for this species, both the band intensities and values for most of the Herman–Wallis coefficients are known up to the sixth overtone[2] ($v = 7 \leftarrow v = 0$). Heretofore, however, analytic theoretical expressions for the treatment of such data have been available only up to the fifth overtone.[3] Recently, we have been able to extend the calculations, by means of computer algebra,[4] to obtain accurate analytic matrix elements including contributions from terms up to eighth order (a_8) in the Dunham potential-energy function[5]

$$V(x) = a_0x^2(1 + \sum_{j=1}^{8} a_jx^j), \tag{1}$$

where $x = (R - R_e)/R_e$ is the reduced displacement from the equilibrium internuclear separation. Utilizing these matrix elements, we have generated accurate expressions for the two Herman–Wallis coefficients C_0^7 and D_0^7 for the sixth overtone, and an additional correction term (smaller than the leading term by a factor of order $\gamma = 2B_e/\omega_e \simeq 10^{-2}$) for C_0^6. These results are discussed in the following section.

In Section 3, after reviewing previous results for the extraction of the dipole-moment function from measured intensities, we fit simultaneously all the data (i.e. vibrational dipole-moment matrix elements, the relative signs of which are chosen to give the best overall rotational dependence as expressed through the Herman–Wallis coefficients) and obtain a value for M_7 in the series expansion of the dipole-moment function

$$M(x) = \sum_{j=1}^{7} M_jx^j \tag{2}$$

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for HCl. This value is then used in order to refine the representation in terms of the Padé approximant[1]

$$M(x) = \frac{[M_0(1+x)^3]}{(1 + \sum_{j=1}^{7} e_j x^j)} \tag{3}$$

The latter form is useful for extrapolation because it has built into it the correct long- and short-range asymptotic dependences and limits.

2. HERMAN–WALLIS COEFFICIENTS

The Herman–Wallis coefficients[6] C_0^v and D_0^v are defined according to the expression

$$F_0^v(m) \equiv \frac{\langle 0J|M(x)|vJ'\rangle^2}{\langle 00|M(x)|v0\rangle^2} = 1 + C_0^v m + D_0^v m^2 + \cdots, \tag{4}$$

in which

$$m = \frac{[J'(J'+1) - J(J+1)]}{2} \tag{5}$$

and v, J denote the usual vibrational and rotational quantum numbers, respectively. With the dipole-moment function expressed in the form (2), the coefficients C_0^v and D_0^v involve matrix elements of powers of x which, in turn, can be expressed as rapidly converging expansions in terms of the Dunham a_j and the expansion parameter[7] γ. Through the use of computer algebra, we have extended our previous results[8] for these matrix elements to include all terms up to order a_1^8 (a_1a_7, a_8, etc.) for the vibrational states $0 \leq v \leq 7$. These new results are consistent with the accuracy of the Dunham potential itself, because at present only the coefficients a_1–a_7 have been determined with statistical significance[9] from wavenumber data over the same range of vibrational states. (Although the coefficient a_8 is effectively zero, other eighth-order terms, e.g. a_1^8, are important in determining the numerical values for C_0^7 and D_0^7.)

The new analytic expressions for C_0^7 and D_0^7, written in terms of variables

$$\delta_j = 3\gamma^3\sqrt{5}M_j/2\langle 0|M(x)|6\rangle \tag{6}$$

and

$$\lambda_j = 3\gamma^{7/2}\sqrt{70}M_j/4\langle 0|M(x)|7\rangle, \tag{7}$$

are presented in the Appendix along with the correction term to C_0^6. Numerical values for HCl will be compared with experimental values in the next section.

3. THE DIPOLE-MOMENT FUNCTION OF HCl

Intensity measurements and the construction of the dipole-moment function for HCl have long been of interest to both experimentalists and theoreticians; we give here a brief outline of some of the highlights of this research. In 1927, Bourgin[10] made measurements of the fundamental band intensity and deduced the value for $M_1/R_e = 0.828 \times 10^{-10}$ esu. Using the currently accepted equilibrium separation, this implies a value for M_1 of 1.06 D. A few years later, Dunham[11] measured the overtone intensities and inferred two possible dipole-moment functions depending on the relative sign of the $\langle 0|M(x)|1\rangle / \langle 0|M(x)|2\rangle$ ratio. Adopting Bourgin's result, and not knowing the permanent dipole moment, he obtained

$$M(x) = M_0 + 1.06x + \begin{Bmatrix} 0.035 \\ 2.28 \end{Bmatrix} x^2. \tag{8}$$

The permanent moment was determined by Rollefson and Rollefson[12] in 1935 from low-resolution refraction measurements; they obtained the value $M_0 = (1.18 \pm 0.05)$ D. An independent determination by Bell and Coop[13] from the temperature dependence of the polarization of HCl yielded the similar value $M_0 = 1.08$ D. Subsequently, Penner and Weber[14] remeasured the band intensities for the fundamental and the first overtone, and derived the dipole-moment function

$$M(x) = M_0 + 1.21x \pm \begin{Bmatrix} 1.96 \\ 0.302 \end{Bmatrix} x^2 \tag{9}$$

Benedict *et al.*,[15] in a systematic study of the individual line strengths for a number of vibrational bands (overtones as well as hot bands) for HCl and DCl, used the rotational dependence of the line strengths to determine the relative signs for M_0 and M_1. By considering both anharmonic-oscillator and Morse wavefunctions and varying the number of terms in the series representation of the dipole-moment function, they derived several functions to fit their data. For example, for the anharmonic oscillator wave functions and a cubic expansion, their results were

$$M(x) = 1.085 + 1.19x - 0.572x^2 - 2.23x^3. \tag{10}$$

Independent measurements and analysis of similar data by Legay[16] about the same time led to the similar though less accurate result

$$M(x) = 1.092 + 1.213x - 0.447x^2. \tag{11}$$

In 1959, Burrus[17] studied the Stark effect in DCl, and deduced the value for the $J = 0 \longrightarrow 1$ pure rotational dipole-moment matrix element of (1.12 ± 0.04) D. The corresponding value for HCl could, in principle, be calculated by considering the zero-point vibrational motion and the breakdown of the Born–Oppenheimer approximation.[18] In 1960, Cashion and Polanyi[19] reported the determination of $M_0/M_1 = 1.12 \pm 0.18$ from the analysis of emission spectra, in fair agreement with the corresponding value obtained from absorption measurements. The Herman–Wallis factor for the first overtone band

$$F_0^2 = 1 - (8.1 \pm 2.2) \times 10^{-3}\ m \tag{12}$$

was reported by Jaffe *et al.*[20] in 1962 from improved refraction spectra.

Beginning in 1967, innovative experimental techniques produced increasingly more accurate dipole-moment data. Sanderson,[21] using Fourier spectroscopy, measured the strengths of a number of lines in the pure rotational band. In 1970, Kaiser[22] reported very accurate molecular-beam electric-resonance data for HCl and DCl, and derived the following expression for the dipole-moment function:

$$\begin{aligned} M(x) = 1.0933 \pm 0.0005 + (1.179 \pm 0.025)x + (0.13 \pm 0.09)x^2 \\ - (1.32 \pm 0.31)x^3 - (1.02 \pm 0.49)x^4. \end{aligned} \tag{13}$$

In the same year, Toth *et al.*[23] published analytic expressions for the C_0^v and D_0^v coefficients for $v = 1 \longrightarrow 3$ and calculated the dipole-moment series

$$M(x) = 1.095 + (1.15 \pm 0.02)x - (0.107 \pm 0.041)x^2 - (1.5 \pm 0.14)x^3. \tag{14}$$

Reanalyses of the existing data, using numerical[24] and more accurate analytic results[25] for the matrix elements, led to

$$M(x) = 1.0935 \pm 0.0007 + (1.21 \pm 0.03)x + (0.024 \pm 0.067)x^2 - (1.69 \pm 0.24)x^3, \tag{15}$$

and

$$M(x) = 1.09323 + 1.2069x + 0.02386x^2 - 1.673x^3 + 1.6x^4. \tag{16}$$

Table 1. Experimental potential-energy parameters and rotationless dipole-moment matrix elements.

j	a_j	$\langle 0\lvert M(x)\rvert j\rangle$/debye
1	$-2.3633725 \pm 3.5 \times 10^{-5}$	$7.12 \times 10^{-2} \pm 2.5 \times 10^{-3}$
2	$3.6605756 \pm 1.9 \times 10^{-4}$	$-7.75 \times 10^{-3} \pm 2.5 \times 10^{-4}$
3	$-4.74921 \pm 1.3 \times 10^{-3}$	$5.15 \times 10^{-4} \pm 2.0 \times 10^{-5}$
4	$5.4529 \pm 9.9 \times 10^{-3}$	$-3.063 \times 10^{-5} \pm 1.0 \times 10^{-7}$
5	$-5.516 \pm 3.2 \times 10^{-2}$	$-8.42 \times 10^{-6} \pm 3.6 \times 10^{-8}$
6	4.284 ± 0.13	$6.61 \times 10^{-6} \pm 2.4 \times 10^{-8}$
7	-1.73 ± 0.42	$-3.27 \times 10^{-6} \pm 1.1 \times 10^{-8}$
8	-0.03 ± 0.39	—
	$\gamma = 7.083694 \times 10^{-3} \pm 1.7 \times 10^{-8}$	$\langle 0\lvert M(x)\rvert 0\rangle = 1.10857 \pm 3 \times 10^{-4}$†

† The quantity actually reported in Ref. 29 was $\lvert\langle 01\lvert M(x)\rvert 01\rangle\rvert = 1.1086 \pm 0.0003$ D; this value has been corrected by terms of order γ to yield $\lvert\langle 0\lvert M(x)\rvert 0\rangle\rvert$ that, by convention, we regard as positive.

A remeasurement and analysis of the 3 ← 0 intensities by Niay *et al.*[26] again led to the similar function

$$M(x) = 1.093 + 1.2069x + 0.0227x^2 - 1.676x^3. \tag{17}$$

In a more recent study by Ogilvie *et al.*,[27] including the results for the 4 ← 0 and 5 ← 0 dipole-moment matrix elements,[2] a six-term dipole-moment function was derived, *viz.*

$$M(x) = 1.09333 + 1.20597x + 0.0399x^2 - 1.6349x^3 - 0.700x^4 + 5.011x^5. \tag{18}$$

In addition, these authors reported accurate *ab initio* calculations of the dipole-moment function at large internuclear separations that enabled them to model the dipole-moment function in terms of the Padé approximant given in Eq. (3).

Finally, Tipping and Ogilvie[3] used the 6 ← 0 experimental results[2] in order to derive the seven-term expansion

$$M(x) = 1.09333 \pm 0.00086 + (1.20538 \pm 0.039)x + (0.03842 \pm 0.060)x^2 - (1.4882 \pm 0.10)x^3 - (0.9881 \pm 0.14)x^4 - (0.6476 \pm 0.19)x^5 - (0.9358 \pm 0.41)x^6. \tag{19}$$

In the present paper, we have extended our analysis, including the 7 ← 0 dipole data[2] in order to derive an additional term M_7 in Eq. (2) for HCl. The experimental data, namely the potential-energy parameters[9] a_j and rotationless dipole-moment matrix elements[2,3] used as input in this analysis are given in Table 1, and the resulting dipole-moment coefficients in Table 2. As already mentioned, the relative signs of these matrix elements are chosen to give the best overall fit for the rotational dependence as reflected in the Herman–Wallis coefficients, and the comparison between the theoretical and experimental C_0^v and D_0^v coefficients is presented in Table 3. The estimated uncertainties

Table 2. Dipole-moment function coefficients M_j (in debye) and Padé parameters e_j.

	Series [Eq. (2)]		Padé [Eq. (3)]
M_0	1.09343 ± 0.00075	M_0	1.09343 ± 0.00075
M_1	1.20538 ± 0.039	e_1	1.89762 ± 0.036
M_2	0.03842 ± 0.058	e_2	0.87296 ± 0.095
M_3	-1.4882 ± 0.098	e_3	1.3321 ± 0.17
M_4	-0.9878 ± 0.15	e_4	1.9871 ± 0.30
M_5	-0.6475 ± 0.19	e_5	1.2573 ± 0.49
M_6	-0.946 ± 0.23	e_6	3.1344 ± 0.74
M_7	0.021 ± 0.50	e_7	2.5470 ± 1.2

Table 3. Comparison of calculated and measured Herman–Wallis coefficients.

	Experiment	Theory
C_0^0	—	0
D_0^0	—	$1.1 \times 10^{-4} \pm 3.6 \times 10^{-6}$
C_0^1	$-2.60 \times 10^{-2} \pm 2.0 \times 10^{-3}$	$-2.66 \times 10^{-2} \pm 9.1 \times 10^{-4}$
D_0^1	$4.5 \times 10^{-4} \pm 2.0 \times 10^{-4}$	$2.8 \times 10^{-4} \pm 7.6 \times 10^{-6}$
C_0^2	$-8.60 \times 10^{-3} \pm 1.5 \times 10^{-3}$	$-5.67 \times 10^{-3} \pm 7.8 \times 10^{-4}$
D_0^2	$4.1 \times 10^{-4} \pm 2.0 \times 10^{-4}$	$3.1 \times 10^{-4} \pm 8.4 \times 10^{-6}$
C_0^3	1.70×10^{-2}	$1.07 \times 10^{-2} \pm 2.2 \times 10^{-3}$
D_0^3	—	$3.7 \times 10^{-4} \pm 1.9 \times 10^{-5}$
C_0^4	$2.77 \times 10^{-2} \pm 1.1 \times 10^{-3}$	$1.20 \times 10^{-2} \pm 7.2 \times 10^{-3}$
D_0^4	$1.42 \times 10^{-3} \pm 1.7 \times 10^{-4}$	$7.9 \times 10^{-4} \pm 2.7 \times 10^{-5}$
C_0^5	$1.74 \times 10^{-2} \pm 1.3 \times 10^{-3}$	$3.21 \times 10^{-2} \pm 7.0 \times 10^{-3}$
D_0^5	$4.61 \times 10^{-4} \pm 2.4 \times 10^{-4}$	$1.4 \times 10^{-3} \pm 2.7 \times 10^{-4}$
C_0^6	$3.35 \times 10^{-2} \pm 1.1 \times 10^{-3}$	$3.27 \times 10^{-2} \pm 2.8 \times 10^{-3}$
D_0^6	$7.99 \times 10^{-4} \pm 1.8 \times 10^{-4}$	$1.3 \times 10^{-3} \pm 1.1 \times 10^{-4}$
C_0^7	$4.37 \times 10^{-2} \pm 1.3 \times 10^{-3}$	$3.78 \times 10^{-2} \pm 2.4 \times 10^{-3}$
D_0^7	—	$1.6 \times 10^{-3} \pm 5.7 \times 10^{-4}$

in Tables 2 and 3 represent in each case one standard deviation, resulting from the uncertainties in the input parameters given in Table 1, as calculated by a Monte-Carlo method for error propagation.[28] As can be seen from these results, the addition of an extra term in the dipole-moment function does not change the lower coefficients significantly; furthermore, the good overall fit to the Herman–Wallis coefficients attests to the stability of the method and the accuracy of these results.

The series representation of the dipole-moment function, however, has a serious drawback (i.e. it rapidly diverges outside the range of separations in which it was determined) that limits its use for the calculation of higher overtone or hot band intensities. To circumvent this problem, one can use the form (3) that has the proper

Table 4. Dipole-moment function representations for HCl (in debye).

$R/10^{-10}$ m	Series	Padé	MCSCF
0.90	0.774	0.774	0.867
1.0	0.848	0.848	0.937
1.1	0.932	0.932	1.012
1.2	1.023	1.023	1.089
1.25	1.070	1.070	1.127
1.275	1.094	1.094	1.146
1.3	1.117	1.117	1.164
1.35	1.164	1.164	1.198
1.4	1.211	1.211	1.229
1.5	1.298	1.298	1.280
1.6	1.374	1.374	1.312
1.7	1.428	1.429	1.320
1.8	1.452	1.455	1.301
2.0	1.343	1.386	1.181
2.2	0.878	1.151	0.968
2.4	−0.224	0.838	0.718
2.7	−4.07	0.450	0.396
3.0	−12.8	0.232	0.199
3.4	−39.3	0.102	0.077
3.9	−120	0.042	0.027
4.4		0.020	0.012
5.0		0.0094	0.0062
6.0		0.0034	0.0028
7.0		0.0015	0.0014
8.5		0.00055	0.00063
10.0		0.00025	0.00033
13.0		0.00007	0.00011
16.0		0.00003	0.00005

limiting behavior as $R \rightarrow 0$ and $R \rightarrow \infty$, and that also contains eight adjustable parameters. These values (M_0 and e_j, $1 \leq j \leq 7$) can be obtained exactly in terms of the M_j and the results are given in the second column of Table 2. As a result, there are now no free parameters in the Padé form by which the long-range behavior can be quantitatively adjusted. The comparison between series, Padé, and MCSCF dipole-moment functions[27] is presented in Table 4 for a range of R. From these results, one can see that the Padé and MCSCF dipole-moment functions intersect near $R = 7 \times 10^{-10}$ m. However, because the coefficient e_7 is relatively insensitive to the function $M(x)$ over the range in which it is constrained by the experimental data and because its corresponding uncertainty is large, it is possible to modify the value of e_7 slightly so as to make the resulting function fit closely the MCSCF *ab initio* values at other separations.

The range of applicability of the series representation derived from experimental data can be taken to be approximately the range between the classical turning points for the $v = 7$ state; that is $0.98 \leq R/10^{-10}$ m ≤ 1.92. The Padé function coincides with the series representation in this range, and closely approximates the MCSCF results at larger separations. As noted previously,[27] in the intervening region ($0.2 \leq R/10^{-9}$ m ≤ 1.0), the results in Table 4 show that the values of either Padé representation are larger than those computed *ab initio;* this reflects in part the fact that the values for the series $M(x)$ are also larger than the MCSCF values in the range $1.5 \leq R/10^{-10}$ m ≤ 1.8, in which overlap of the data permits a direct comparison. In conclusion, we feel that the dipole-moment function expressed in the form of our Padé approximant is the best available at present, and should have quantitative significance throughout the entire range of internuclear separations $R > 0.9 \times 10^{-10}$ m.

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APPENDIX: HERMAN-WALLIS COEFFICIENTS

(Correction term for C_0^6 and expressions for C_0^7 and D_0^7)

$$C_0^6 = \gamma\ [\ \cdot\ \cdot\ \cdot\ ] + \gamma^2\ [\ (\ - \frac{2751}{8192} a_1^7 + \frac{81165}{8192} a_1^6 - \frac{6503}{2048} a_1^5 a_2 - \frac{8617}{128} a_1^5 + \frac{42357}{2048} a_1^4 a_2$$

$$- \frac{105}{16} a_1^4 a_3 + \frac{38605}{256} a_1^4 + \frac{1099}{512} a_1^3 a_2^2 + \frac{595}{16} a_1^3 a_2 + \frac{5075}{256} a_1^3 a_3 - \frac{2821}{640} a_1^3 a_4 - \frac{2695}{32} a_1^3$$

$$- \frac{24465}{512} a_1^2 a_2^2 + \frac{2667}{320} a_1^2 a_2 a_3 - \frac{8295}{32} a_1^2 a_2 - \frac{189}{16} a_1^2 a_3 - \frac{105}{128} a_1^2 a_4 + \frac{81}{160} a_1^2 a_5 - \frac{1617}{32} a_1^2$$

$$+ \frac{539}{128} a_1 a_2^3 + \frac{931}{8} a_1 a_2^2 - \frac{1827}{64} a_1 a_2 a_3 + \frac{1373}{160} a_1 a_2 a_4 + \frac{1995}{8} a_1 a_2 - \frac{51}{32} a_1 a_3^2 + \frac{385}{8} a_1 a_3$$

$$- \frac{77}{10} a_1 a_4 + \frac{21}{16} a_1 a_5 - \frac{1}{8} a_1 a_6 - \frac{945}{128} a_2^3 + \frac{149}{80} a_2^2 a_3 - \frac{735}{16} a_2^2 - \frac{119}{20} a_2 a_3 - \frac{63}{32} a_2 a_4$$

$$+ \frac{37}{40} a_2 a_5 - \frac{147}{8} a_2 + \frac{245}{32} a_3^2 - \frac{11}{4} a_3 a_4 - 70\ a_3 + \frac{105}{4} a_4 - \frac{56}{5} a_5 + \frac{35}{8} a_6 - \frac{6}{5} a_7$$

$$+ 42\ )\ \delta_0 + (\ - \frac{34923}{2048} a_1^6 + \frac{20559}{256} a_1^5 - \frac{22351}{512} a_1^4 a_2 - \frac{6559}{40} a_1^4 - \frac{29169}{640} a_1^3 a_2 - \frac{29169}{640} a_1^3 a_3$$

$$+ \frac{11247}{128} a_1^3 + \frac{57183}{640} a_1^2 a_2^2 + \frac{4503}{16} a_1^2 a_2 + \frac{1923}{320} a_1^2 a_3 + \frac{129}{160} a_1^2 a_4 + \frac{1017}{20} a_1^2 - \frac{23913}{160} a_1 a_2^2$$

$$+ \frac{10457}{160} a_1 a_2 a_3 - \frac{8291}{32} a_1 a_2 - \frac{223}{4} a_1 a_3 + \frac{39}{16} a_1 a_4 + \frac{1}{8} a_1 a_5 + \frac{77}{40} a_1 + \frac{2451}{160} a_2^3 + \frac{993}{20} a_2^2$$

$$+ \frac{391}{80} a_2 a_3 + \frac{313}{40} a_2 a_4 + \frac{169}{10} a_2 - \frac{129}{8} a_3^2 + \frac{303}{4} a_3 - \frac{163}{5} a_4 + \frac{279}{20} a_5 - \frac{93}{10} a_6$$

$$- \frac{216}{5}\ )\ \delta_1 + (\ - \frac{16429}{128} a_1^5 + \frac{23513}{128} a_1^4 + \frac{9163}{192} a_1^3 a_2 - \frac{9275}{96} a_1^3 - \frac{22785}{64} a_1^2 a_2 - \frac{1589}{64} a_1^2 a_3$$

$$- \frac{3185}{64} a_1^2 + \frac{3829}{16} a_1 a_2^2 + \frac{2149}{8} a_1 a_2 + \frac{693}{16} a_1 a_3 - \frac{343}{40} a_1 a_4 - \frac{21}{4} a_1 - \frac{1029}{16} a_2^2 - \frac{973}{240} a_2 a_3$$

$$- \frac{665}{48} a_2 - \frac{175}{2} a_3 + \frac{259}{8} a_4 - \frac{1337}{60} a_5 + \frac{539}{12}\ )\ \delta_2 + (\ - \frac{37863}{128} a_1^4 + \frac{4473}{64} a_1^3 + \frac{3759}{8} a_1^2 a_2$$

$$+ \frac{777}{20} a_1^2 - \frac{28917}{80} a_1 a_2 - \frac{1533}{20} a_1 a_3 + \frac{49}{4} a_1 + \frac{3927}{40} a_2^2 + \frac{21}{5} a_2 + \frac{1687}{20} a_3 - \frac{469}{10} a_4$$

$$- \frac{238}{5}\ )\ \delta_3 + (\ - \frac{5817}{32} a_1^3 - \frac{4389}{32} a_1^2 + \frac{3745}{8}\ a_1 a_2 - 35\ a_1 - \frac{315}{8} a_2 - \frac{231}{2} a_3 + \frac{105}{2}\ )\ \delta_4$$

$$+ (\ \frac{623}{8} a_1^2 - \frac{245}{4} a_1 + \frac{329}{6} a_2 - \frac{196}{3}\ )\ \delta_5 + (\ \frac{63}{2} a_1 + \frac{63}{2}\ )\ \delta_6 - 42\ \delta_7\ ]$$

$$C_0^7 = \gamma\ [\ (\ - \frac{1}{1024} a_1^6 + \frac{3}{64} a_1^5 - \frac{5}{256} a_1^4 a_2 - \frac{9}{16} a_1^4 + \frac{3}{8} a_1^3 a_2 - \frac{13}{192} a_1^3 a_3 + \frac{75}{28} a_1^3 - \frac{3}{64} a_1^2 a_2^2$$

$$- \frac{27}{14} a_1^2 a_2 + \frac{4}{7} a_1^2 a_3 - \frac{149}{1120} a_1^2 a_4 - \frac{165}{28} a_1^2 + \frac{9}{28} a_1 a_2^2 - \frac{181}{1680} a_1 a_2 a_3 + \frac{25}{7} a_1 a_2 - \frac{19}{14} a_1 a_3$$

$$+ \frac{69}{140} a_1 a_4 - \frac{9}{70} a_1 a_5 + 6\ a_1 - \frac{1}{112} a_2^3 - \frac{3}{7} a_2^2 + \frac{17}{70} a_2 a_3 - \frac{3}{56} a_2 a_4 - \frac{15}{7} a_2 - \frac{5}{252} a_3^2$$

$$+ \frac{20}{21} a_3 - \frac{3}{7} a_4 + \frac{6}{35} a_5 - \frac{1}{21} a_6 - \frac{16}{7}) \lambda_0 + (- \frac{21}{256} a_1^5 + \frac{175}{256} a_1^4 - \frac{35}{48} a_1^3 a_2 - \frac{707}{240} a_1^3$$

$$+ \frac{49}{20} a_1^2 a_2 - \frac{203}{160} a_1^2 a_3 + \frac{199}{32} a_1^2 - \frac{161}{240} a_1 a_2^2 - \frac{241}{60} a_1 a_2 + \frac{443}{240} a_1 a_3 - \frac{49}{40} a_1 a_4 - \frac{31}{5} a_1 + \frac{9}{16} a_2^2$$

$$- \frac{203}{360} a_2 a_3 + \frac{55}{24} a_2 - \frac{10}{9} a_3 + \frac{5}{8} a_4 - \frac{7}{15} a_5 + \frac{7}{3}) \lambda_1 + (- \frac{35}{32} a_1^4 + \frac{7}{2} a_1^3 - \frac{49}{12} a_1^2 a_2 - \frac{203}{30} a_1^2$$

$$+ \frac{49}{10} a_1 a_2 - \frac{191}{60} a_1 a_3 + \frac{13}{2} a_1 - \frac{29}{30} a_2^2 - \frac{38}{15} a_2 + \frac{7}{5} a_3 - \frac{11}{10} a_4 - \frac{12}{5}) \lambda_2 + (- \frac{21}{4} a_1^3$$

$$+ \frac{63}{8} a_1^2 - \frac{15}{2} a_1 a_2 - 7 a_1 + 3 a_2 - \frac{13}{6} a_3 + \frac{5}{2}) \lambda_3 + (- \frac{45}{4} a_1^2 + 8 a_1 - \frac{13}{3} a_2 - \frac{8}{3}) \lambda_4$$

$$+ (- 11 a_1 + 3) \lambda_5 - 4 \lambda_6] + \gamma^2 [- \frac{927}{8192} a_1^8 + \frac{4827}{1024} a_1^7 - \frac{901}{512} a_1^6 a_2 - \frac{12129}{256} a_1^6$$

$$+ \frac{5967}{256} a_1^5 a_2 - \frac{4153}{768} a_1^5 a_3 + \frac{5645}{32} a_1^5 - \frac{213}{256} a_1^4 a_2^2 - \frac{2829}{64} a_1^4 a_2 + \frac{2137}{64} a_1^4 a_3 - \frac{4927}{640} a_1^4 a_4$$

$$- \frac{8235}{32} a_1^4 - \frac{1743}{64} a_1^3 a_2^2 + \frac{1211}{480} a_1^3 a_2 a_3 - \frac{655}{4} a_1^3 a_2 - \frac{97}{2} a_1^3 a_3 + \frac{72}{5} a_1^3 a_4 - \frac{4121}{1120} a_1^3 a_5$$

$$+ 84 a_1^3 + \frac{147}{32} a_1^2 a_2^3 + \frac{2781}{16} a_1^2 a_2^2 - \frac{1809}{40} a_1^2 a_2 a_3 + \frac{6729}{560} a_1^2 a_2 a_4 + \frac{2025}{4} a_1^2 a_2 - \frac{1261}{1008} a_1^2 a_3^2$$

$$+ \frac{215}{6} a_1^2 a_3 + \frac{3}{5} a_1^2 a_4 - \frac{66}{35} a_1^2 a_5 + \frac{235}{336} a_1^2 a_6 + \frac{496}{7} a_1^2 - \frac{411}{16} a_1 a_2^3 + \frac{4439}{560} a_1 a_2^2 a_3$$

$$- \frac{495}{2} a_1 a_2^2 + \frac{313}{5} a_1 a_2 a_3 - \frac{435}{14} a_1 a_2 a_4 + \frac{2437}{280} a_1 a_2 a_5 - 348 a_1 a_2 + \frac{809}{84} a_1 a_3^2$$

$$- \frac{323}{112} a_1 a_3 a_4 - \frac{1445}{14} a_1 a_3 + \frac{171}{7} a_1 a_4 - \frac{264}{35} a_1 a_5 + \frac{16}{7} a_1 a_6 - \frac{71}{140} a_1 a_7 + \frac{144}{7} a_1$$

$$+ \frac{17}{32} a_2^4 + \frac{81}{4} a_2^3 - \frac{197}{28} a_2^2 a_3 + \frac{17}{8} a_2^2 a_4 + \frac{975}{14} a_2^2 - \frac{9}{16} a_2 a_3^2 + \frac{136}{7} a_2 a_3 + \frac{6}{7} a_2 a_4$$

$$- \frac{12}{7} a_2 a_5 + \frac{19}{28} a_2 a_6 + \frac{96}{7} a_2 - \frac{404}{21} a_3^2 + \frac{151}{14} a_3 a_4 - \frac{209}{84} a_3 a_5 + 100 a_3 - \frac{95}{112} a_4^2$$

$$- \frac{285}{7} a_4 + \frac{136}{7} a_5 - \frac{64}{7} a_6 + \frac{132}{35} a_7 - \frac{15}{14} a_8 - \frac{360}{7}) \lambda_0 + (- \frac{16935}{2048} a_1^7 + \frac{117227}{2048} a_1^6$$

$$- \frac{72781}{1536} a_1^5 a_2 - \frac{185627}{960} a_1^5 + \frac{146623}{2560} a_1^4 a_2 - \frac{73537}{960} a_1^4 a_3 + \frac{242423}{896} a_1^4 + \frac{94333}{1920} a_1^3 a_2^2$$

$$+ \frac{37157}{210} a_1^3 a_2 + \frac{782447}{13440} a_1^3 a_3 - \frac{17743}{448} a_1^3 a_4 - \frac{48513}{560} a_1^3 - \frac{1003557}{4480} a_1^2 a_2^2 + \frac{1012829}{10080} a_1^2 a_2 a_3$$

$$- \frac{89497}{168} a_1^2 a_2 - \frac{5155}{126} a_1^2 a_3 - \frac{26399}{2240} a_1^2 a_4 + \frac{8401}{1680} a_1^2 a_5 - \frac{16991}{240} a_1^2 + \frac{60281}{1120} a_1 a_2^3$$

$$+ \frac{38643}{140} a_1 a_2^2 - \frac{21031}{224} a_1 a_2 a_3 + \frac{9101}{112} a_1 a_2 a_4 + \frac{49939}{140} a_1 a_2 - \frac{10279}{504} a_1 a_3^2 + \frac{12443}{112} a_1 a_3$$

$$- \frac{4393}{140} a_1 a_4 + \frac{839}{280} a_1 a_5 - \frac{1007}{420} a_1 a_6 - \frac{794}{35} a_1 - \frac{855}{32} a_2^3 + \frac{721}{40} a_2^2 a_3 - \frac{585}{8} a_2^2$$

$$- \frac{143}{6} a_2a_3 - \frac{69}{16} a_2a_4 + \frac{469}{60} a_2a_5 - \frac{49}{4} a_2 + \frac{413}{16} a_3^2 - \frac{203}{8} a_3a_4 - \frac{631}{6} a_3 + \frac{365}{8} a_4$$

$$- \frac{77}{3} a_5 + \frac{49}{4} a_6 - \frac{91}{10} a_7 + \frac{105}{2}) \lambda_1 + (- \frac{47623}{512} a_1^6 + \frac{28801}{128} a_1^5 - \frac{43997}{384} a_1^4a_2$$

$$- \frac{70561}{240} a_1^4 - \frac{18297}{80} a_1^3a_2 - \frac{7219}{60} a_1^3a_3 + \frac{642}{7} a_1^3 + \frac{58143}{160} a_1^2a_2^2 + \frac{39899}{70} a_1^2a_2$$

$$+ \frac{7477}{420} a_1^2 a_3 + \frac{447}{140} a_1^2a_4 + \frac{2444}{35} a_1^2 - \frac{19577}{56} a_1a_2^2 + \frac{50833}{315} a_1a_2a_3 - \frac{7715}{21} a_1a_2$$

$$- \frac{8231}{63} a_1a_3 + \frac{2187}{140} a_1a_4 - \frac{1034}{105} a_1a_5 + \frac{388}{15} a_1 + \frac{7855}{168} a_2^3 + \frac{1609}{21} a_2^2 + \frac{1391}{70} a_2a_3$$

$$+ \frac{223}{21} a_2a_4 + \frac{344}{35} a_2 - \frac{2749}{63} a_3^2 + \frac{2383}{21} a_3 - \frac{5822}{105} a_4 + \frac{906}{35} a_5 - \frac{2176}{105} a_6 - \frac{1888}{35}) \lambda_2$$

$$+ (- \frac{45395}{128} a_1^5 + \frac{40047}{128} a_1^4 + \frac{4439}{16} a_1^3a_2 - \frac{539}{5} a_1^3 - \frac{59019}{80} a_1^2a_2 - \frac{8161}{120} a_1^2a_3 - \frac{131}{2} a_1^2$$

$$+ \frac{21089}{40} a_1a_2^2 + \frac{1862}{5} a_1a_2 + \frac{4123}{40} a_1a_3 - \frac{147}{4} a_1a_4 - \frac{156}{5} a_1 - \frac{825}{8} a_2^2 - \frac{383}{15} a_2a_3$$

$$- 5 a_2 - \frac{392}{3} a_3 + \frac{207}{4} a_4 - \frac{196}{5} a_5 + 56) \lambda_3 + (- \frac{16741}{32} a_1^4 + \frac{115}{4} a_1^3 + \frac{11473}{12} a_1^2a_2$$

$$+ \frac{628}{15} a_1^2 - \frac{2649}{5} a_1a_2 - \frac{5159}{30} a_1a_3 + 42 a_1 + \frac{1531}{10} a_2^2 - \frac{48}{5} a_2 + \frac{616}{5} a_3 - \frac{369}{5} a_4$$

$$- \frac{296}{5}) \lambda_4 + (- \frac{1557}{8} a_1^3 - \frac{1669}{8} a_1^2 + \frac{4073}{6} a_1a_2 - \frac{226}{3} a_1 - \frac{81}{2} a_2 - \frac{505}{3} a_3 + 65) \lambda_5$$

$$+ (130 a_1^2 - 54 a_1 + 56 a_2 - 80) \lambda_6 + (14 a_1 + 42) \lambda_7 - 56 \lambda_8]$$

$$D_0^7 = [\frac{1}{2} C_0^7]^2 + \gamma^2 [(\frac{3}{128} a_1^5 - \frac{85}{128} a_1^4 + \frac{5}{24} a_1^3a_2 + \frac{641}{120} a_1^3 - \frac{49}{20} a_1^2a_2 + \frac{29}{80} a_1^2a_3$$

$$- \frac{1377}{80} a_1^2 + \frac{23}{120} a_1a_2^2 + \frac{113}{15} a_1a_2 - \frac{227}{120} a_1a_3 + \frac{7}{20} a_1a_4 + \frac{237}{10} a_1 - \frac{23}{40} a_2^2 + \frac{29}{180} a_2a_3$$

$$- \frac{131}{20} a_2 + \frac{97}{45} a_3 - \frac{13}{20} a_4 + \frac{2}{15} a_5 - \frac{58}{5}) \lambda_0 + (- \frac{651}{8192} a_1^7 - \frac{651}{8192} a_1^6 - \frac{2667}{2048} a_1^5a_2$$

$$- \frac{21}{256} a_1^5 - \frac{2835}{2048} a_1^4a_2 - \frac{959}{256} a_1^4a_3 + \frac{455}{512} a_1^4 - \frac{889}{512} a_1^3a_2^2 - \frac{35}{32} a_1^3a_2 - \frac{2093}{512} a_1^3a_3$$

$$- \frac{6673}{1280} a_1^3a_4 - \frac{385}{64} a_1^3 - \frac{1449}{512} a_1^2a_2^2 - \frac{569}{640} a_1^2a_2a_3 + \frac{245}{64} a_1^2a_2 - \frac{91}{32} a_1^2a_3 - \frac{8493}{1280} a_1^2a_4$$

$$- \frac{577}{320} a_1^2a_5 + \frac{1463}{80} a_1^2 + \frac{111}{128} a_1a_2^3 - \frac{21}{16} a_1a_2^2 - \frac{3439}{640} a_1a_2a_3 + \frac{1241}{320} a_1a_2a_4 - \frac{433}{48} a_1a_2$$

$$+ \frac{53}{48} a_1a_3^2 + \frac{1801}{480} a_1a_3 - \frac{149}{40} a_1a_4 - \frac{81}{16} a_1a_5 + \frac{89}{40} a_1a_6 - \frac{1471}{60} a_1 - \frac{57}{128} a_2^3 + \frac{949}{480} a_2^2a_3$$

$$+ \frac{1459}{1440} a_2^2 - \frac{181}{120} a_2a_3 - \frac{135}{64} a_2a_4 + \frac{249}{80} a_2a_5 + \frac{323}{45} a_2 - \frac{25}{32} a_3^2 + \frac{85}{48} a_3a_4 - \frac{173}{60} a_3$$

$$+ \frac{131}{80} a_4 - \frac{9}{5} a_5 - \frac{11}{8} a_6 + \frac{3}{2} a_7 + \frac{2129}{180}) \lambda_1 + (- \frac{2261}{1024} a_1^6 - \frac{567}{256} a_1^5 - \frac{3269}{256} a_1^4 a_2$$

$$- \frac{35}{16} a_1^4 - \frac{483}{32} a_1^3 a_2 - \frac{2717}{192} a_1^3 a_3 + \frac{63}{8} a_1^3 + \frac{9}{64} a_1^2 a_2^2 - \frac{21}{2} a_1^2 a_2 - 19 a_1^2 a_3 - \frac{641}{160} a_1^2 a_4$$

$$- \frac{41}{2} a_1^2 - \frac{171}{16} a_1 a_2^2 + \frac{3011}{240} a_1 a_2 a_3 + \frac{77}{6} a_1 a_2 - \frac{32}{3} a_1 a_3 - \frac{207}{16} a_1 a_4 + \frac{113}{20} a_1 a_5$$

$$+ \frac{779}{30} a_1 + \frac{49}{16} a_2^3 - 3 a_2^2 - \frac{51}{8} a_2 a_3 + \frac{67}{8} a_2 a_4 - \frac{42}{5} a_2 + \frac{107}{36} a_3^2 + \frac{9}{2} a_3 - \frac{23}{5} a_4 - \frac{33}{10} a_5$$

$$+ \frac{53}{15} a_6 - \frac{61}{5}) \lambda_2 + (- \frac{4263}{256} a_1^5 - \frac{4347}{256} a_1^4 - \frac{951}{32} a_1^3 a_2 - \frac{63}{4} a_1^3 - \frac{1539}{32} a_1^2 a_2 - \frac{187}{32} a_1^2 a_3$$

$$+ \frac{207}{8} a_1^2 + \frac{333}{16} a_1 a_2^2 - 27 a_1 a_2 - \frac{855}{32} a_1 a_3 + \frac{921}{80} a_1 a_4 - \frac{115}{4} a_1 - \frac{135}{16} a_2^2 + \frac{187}{10} a_2 a_3$$

$$+ \frac{67}{6} a_2 - \frac{19}{2} a_3 - \frac{99}{16} a_4 + \frac{129}{20} a_5 + \frac{77}{6}) \lambda_3 + (- \frac{99}{2} a_1^4 - \frac{855}{16} a_1^3 + \frac{9}{4} a_1^2 a_2 - 45 a_1^2$$

$$- \frac{225}{4} a_1 a_2 + \frac{47}{2} a_1 a_3 + 35 a_1 + 23 a_2^2 - 20 a_2 - 11 a_3 + 11 a_4 - 14) \lambda_4$$

$$+ (- \frac{1875}{32} a_1^3 - \frac{2475}{32} a_1^2 + \frac{475}{8} a_1 a_2 - 55 a_1 - \frac{165}{8} a_2 + \frac{115}{6} a_3 + \frac{33}{2}) \lambda_5 + (- \frac{33}{4} a_1^2$$

$$- \frac{99}{2} a_1 + 39 a_2 - 24) \lambda_6 + (\frac{63}{2} a_1 - \frac{21}{2}) \lambda_7 + 16 \lambda_8]$$