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ANALYTIC VIBRATIONAL MATRIX ELEMENTS FOR DIATOMIC MOLECULES

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PROGRAM SUMMARY

Title of program: VIBMATEL

Catalogue number: AAFQ

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

Computer for which the program is designed and others on which it is operable: any computer having a FORTRAN-77 compiler and sufficient core

Computer: Sperry 1100/91; *Installation:* P.S.I. Université de Paris-Sud, F-91405 Orsay, France

Operating system: SPERRY OS1100 Exec-8, Level 39R2

Programming language used: FORTRAN-77 with nonstandard IMPLICIT statement

High-speed storage required: 169 Kwords

No. of bits in a word: 36

Overlay structure: optional

Peripherals used: card reader or input console, line printer

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No. of lines in combined program and test deck: 5915

Keywords: molecular, diatomic, vibrational, matrix elements, expectation values, Dunham potential–energy function, rotational dependence

Nature of the physical problem
The vibrational matrix elements and expectation values for a diatomic molecule, including the rotational dependence, are calculated for powers of the reduced displacement in terms of the parameters of the Dunham potential–energy function [1].

Method of solution
Explicit expressions for the matrix elements in terms of the vibrational quantum numbers v and v', or Δv, are given for x^l, $0 \le l \le 8$ or 7, respectively, in two different groups: in one group, $0 \le v \le v' \le 7$ and $0 \le l \le 8$, up to the eighth order in the potential–energy function; in the other group, $0 \le \Delta v = v' - v \le 7$ and $0 \le l \le 7$, up to the sixth order in the potential–energy function.

Typical running time
1.3 s.

Reference
[1] J.F. Ogilvie and R.H. Tipping, Intern. Rev. Phys. Chem 3 (1983) 3.

LONG WRITE-UP

1. Introduction

According to quantum mechanics a matrix element of the corresponding operator is associated with any physically observable quantity. For the comparison between theoretically and experimentally determined properties, one thus requires accurate expectation values or matrix elements. For the evaluation of these quantities, one can use either numerical methods, requiring numerical integration over an appropriate range, or analytic expressions, if the theory to produce the latter has generated an adequate supply of expressions over the necessary range of quantum numbers of the discrete states. The numerical method is rather general, but requires a relatively long calculation for each value, whereas once the analytic expressions have been formed, probably as the result of long calculations, the results are fairly simple expressions that require only brief times for evaluation.

2. Summary of the theory and its implementation

In the program VIBMATEL, we use a series of analytic expressions for the vibration–rotational expectation values and vibrational matrix elements of a diatomic molecule (in a $^1\Sigma$ state) in terms of the parameters of the potential–energy function due to Dunham [1], commonly used in spectroscopic investigations of these molecules:

$$V(x) = B_e\gamma^{-2}x^2\left(1 + \sum_{j=1} a_j x^j\right). \tag{1}$$

The vibration–rotational wavefunctions ψ_{vJ} implicit in the calculations are the solutions of the dimensionless Schrödinger equation

$$\frac{d^2\psi_{vJ}(x)}{dx^2} + \frac{1}{B_e}\left(E_{vJ} - V(x) - \frac{B_e J(J+1)}{(1+x)^2}\right)\psi_{vJ}(x) = 0. \tag{2}$$

Here x is the reduced internuclear displacement in terms of the instantaneous R and equilibrium R_e distances, $x = (R - R_e)/R_e$; B_e is the equilibrium rotational parameter, $B_e = h/(8\pi^2 c\mu R_e^2)$, having the same (wavenumber) units as V; γ is the appropriate dimensionless expansion parameter, the ratio $\gamma = 2B_e/\omega_e$ of limiting rotational and vibrational spectral intervals, that governs the convergence of the analytic expressions to follow. The a_j coefficients are usually determined from the frequencies of lines in the observed vibration–rotational spectra, whether in absorption, emission or Raman scattering.

It is convenient [2] to express various molecular properties, for instance rotational parameters B_v, shielding factors or spectral line intensities, in the form of power-series expansions of the corresponding functions in terms of the reduced displacement x; e.g.

$$M(x) = \sum_{l=0} M_l x^l. \tag{3}$$

In this case, any vibrational matrix element of the function $M(x)$ can easily be expressed in terms of the sum of the corresponding matrix elements of x:

$$\langle v|M(x)|v'\rangle = \sum_{l=0} M_l \langle v|x^l|v'\rangle \tag{4}$$

in which the $\langle v|$ and $|v'\rangle$ correspond to the vibrational eigenfunctions $\psi_{v0}(x)$ and $\psi_{v'0}(x)$. If the values of v and v' are identical, then we have the expectation values of the function $M(x)$ in a particular vibrational state $v = v'$.

Two groups of analytic expressions are used in the program VIBMATEL. In the first group, the expressions are given for explicit values of v and v', in the range $0 \le v \le v' \le 7$, useful for powers of x in the range $0 \le l \le 8$. (Higher powers can be generated from exact recurrence relations [3].) The expressions contain all terms in the potential-energy parameters up to a_8 inclusive. In the second group, the expressions are given in terms of the difference between vibrational quantum numbers, $\Delta v = v' - v$, in the range $0 \le \Delta v \le 7$ for powers of x up to x^7 and contain all terms up to a_6 inclu-

sive. These two groups of expressions have been derived by different methods, that we summarize as follows.

The matrix elements and expectation values in terms of v and v' have been generated [2] entirely by computer algebra [4], through the use of the vibrational wavefunctions [5], $\psi_{v0}(x) = N_v g_v(x)\psi_0(x)$. The derivation of the wavefunctions $\psi_{v0}(x)$ with the aid of quantum-mechanical relations [3] has been described in detail elsewhere [2]. The preexponential functions $g_v(x)$ are polynomials with coefficients involving γ and a_j. Thus, the general vibrational matrix element $\langle v | x^l | v' \rangle$ can be written as

$$\langle v | x^l | v' \rangle = N_v N_{v'} \langle 0 | g_v(x) x^l g_{v'}(x) | 0 \rangle, \tag{5}$$

so all that is required is a method of generating the ground-state ($v = 0$) expectation values of x^l. For the latter purpose, a simple two-term recurrence relation has been previously devised [4]. By this means, all the expectation values and matrix elements in the first group have been evaluated.

The vibrational matrix elements with a functional dependence on v, in the second group, have been evaluated by the application of perturbation theory [6] using the harmonic-oscillator basis set and including the anharmonic-oscillator terms as successive perturbations; these matrix elements have been generated by numerical computer programs. The method has been previously described [7] and some expressions have also been published; the present set of terms extends the treatment.

It is important to confirm that the given expressions are correct. For this purpose some procedures are available. First of all, if all the values of the coefficients a_j are set to zero, the expressions reduce to the harmonic-oscillator results that can be written in closed form. Secondly, the two groups of expressions can be used to check each other, by analytic evaluation of the appropriate differences. Tests have confirmed the correctness of the expressions by this method (and in fact located a few transcription errors). However, some expressions for which overlap between the two groups does not occur could not be checked in this way. The expressions $\langle v | x^8 | v' \rangle$ in the first group are in this category. However, because of the nature of the generation of these expressions, that in no way deviates from the method of generating the expressions for $l < 8$ and that is in fact a trivial extension of the algorithm for which all necessary terms were confirmed to be correct, it is believed that these expressions are also correct. The expressions $\langle v | x^l | v + 7 \rangle$ in the second group could be checked against those in the first group for only the special case $v = 0$. As an alternative method of checking all the matrix elements, one can use a well known potential-energy function, such as that due to Kratzer [2], for which the matrix elements take a simple and calculable form.

It may be desirable to know the rotational dependence of these matrix elements and expectation values, thus in effect to generate the matrix elements $\langle vJ | x^l | v'J \rangle$ that may be off-diagonal in v but diagonal in J. One can achieve this objective in a formal way by using the known J-dependence [2] of the arguments, the parameter a_j and γ. This dependence is in fact expressed in terms of $J(J+1) = \beta$, and consists of a series of terms of the form:

$$\begin{aligned}\gamma(\beta) = \gamma &- \tfrac{3}{2}\gamma^3\beta(a_1 + 1) \\ &+ \tfrac{3}{8}\gamma^5\beta^2\left(15a_1^2 + 30a_1 - 8a_2 + 25\right) \\ &+ \gamma^7\beta^3(\cdots) + \cdots,\end{aligned} \tag{6}$$

$$\begin{aligned}a_j(\beta) = a_j + \gamma^2\beta\Big[&-3a_j(1 + a_1) \\ &+ (j+3)\left(a_j + (-1)^j\right)\Big] \\ &+ \gamma^4\beta^2(\cdots) + \gamma^6\beta^3(\cdots) + \cdots.\end{aligned} \tag{7}$$

Because for almost all known diatomic molecules, the range of γ is $\approx 10^{-2} > \gamma > \approx 10^{-4}$, there is a rapid convergence of these series provided that the values of J are not too large ($J \leq 30$ for $\gamma \approx 10^{-2}$).

All the expressions for $\langle vJ | x^l | v'J \rangle$, $a_j(\beta)$ and $\gamma(\beta)$ have been automatically converted into FORTRAN statements and have then been assembled into ten subroutines. The first eight subroutines contain the statements corresponding to the expressions in the first group $\langle v | x^l | v' \rangle$, $0 \leq v \leq v' \leq 7$, with a different value of v in each subroutine. The ninth subroutine contains the expressions for $\langle v | x^l | v + \Delta v \rangle$ belonging to the second group. The tenth subroutine produces the J-dependent parameters $a_j(\beta)$ and $\gamma(\beta)$ if necessary,

Table 1
Values of contributions of terms containing successive powers of γ to vibrational matrix elements of HCl with $\Delta v = 1$ or 2, as v increases

Matrix element	$\gamma^{3/2}$	$\gamma^{5/2}$	$\gamma^{7/2}$	$\gamma^{9/2}$	Sum
$\langle 0 \mid x^3 \mid 1\rangle$	0.6324×10^{-3}	0.1103×10^{-3}	0.4459×10^{-5}	0.1879×10^{-6}	0.7473×10^{-3}
$\langle 5 \mid x^3 \mid 6\rangle$	0.9294×10^{-2}	0.8880×10^{-2}	0.1945×10^{-2}	0.4214×10^{-3}	0.2054×10^{-1}
$\langle 10 \mid x^3 \mid 11\rangle$	0.2307×10^{-1}	0.4033×10^{-1}	0.1616×10^{-1}	0.6393×10^{-2}	0.8596×10^{-1}
$\langle 15 \mid x^3 \mid 16\rangle$	0.4047×10^{-1}	0.1029	0.5993×10^{-1}	0.3445×10^{-1}	0.2377
Matrix element	γ	γ^2	γ^3	γ^4	Sum
$\langle 0 \mid x^2 \mid 2\rangle$	0.5009×10^{-2}	-0.2250×10^{-3}	-0.1100×10^{-4}	-0.7830×10^{-6}	0.4772×10^{-2}
$\langle 5 \mid x^2 \mid 7\rangle$	0.2295×10^{-1}	-0.4467×10^{-2}	-0.7645×10^{-3}	-0.2213×10^{-3}	0.1750×10^{-1}
$\langle 10 \mid x^2 \mid 12\rangle$	0.4069×10^{-1}	-0.1401×10^{-1}	-0.4203×10^{-2}	-0.2146×10^{-2}	0.2033×10^{-2}
$\langle 15 \mid x^2 \mid 17\rangle$	0.5841×10^{-1}	-0.2886×10^{-1}	-0.1239×10^{-1}	-0.9070×10^{-2}	0.8092×10^{-2}

and is executed before the previous subroutines are called as required. The entire program is thus readily adaptable to an overlay or segmented structure for use in a small core.

The limitations of the validity of the results can be easily ascertained because the analytic expressions are series in powers of γ. As already mentioned, the J-dependence is found by a formal substitution that depends on a rapid convergence of the expressions for $a_j(\beta)$ and $\gamma(\beta)$; the explicit requirement for this convergence is that $J(J+1) \ll \gamma^{-2}$. Another limitation of the use of the expressions for the matrix elements in the first group arises if a complete set of a_j, $1 \le j \le 8$, is unavailable, and correspondingly for a_j $1 \le j \le 6$, in the second group. It is important not simply to use the given expressions with the unknown values of a_j merely set equal to zero. If the set of known a_j terminates at a_k, then all terms (coefficients of γ to some power) that contain any potential-energy coefficients a_j with $j > k$ should be removed from the expressions. An alternative procedure would be to extend the set of known a_j with values appropriate to a particular model potential–energy function (such as that of Morse or Lennard-Jones [2]). The same injunction applies to the expressions $\langle v \mid x^l \mid v + \Delta v\rangle$ for which in most cases a set of a_j, $1 \le j \le 6$, is required. Also in the

Table 2
Description of subroutines of program VIBMATEL

Subroutine name	Input parameters	Output parameters
MEL0	γ, a_1–a_8, v'	$\langle 0 \mid x^l \mid v'\rangle$, $0 \le l \le 8$, $0 \le v' \le 7$
MEL1	γ, a_1–a_8, v'	$\langle 1 \mid x^l \mid v'\rangle$, $0 \le l \le 8$, $1 \le v' \le 7$
MEL2	γ, a_1–a_8, v'	$\langle 2 \mid x^l \mid v'\rangle$, $0 \le l \le 8$, $2 \le v' \le 7$
MEL3	γ, a_1–a_8, v'	$\langle 3 \mid x^l \mid v'\rangle$, $0 \le l \le 8$, $3 \le v' \le 7$
MEL4	γ, a_1–a_8, v'	$\langle 4 \mid x^l \mid v'\rangle$, $0 \le l \le 8$, $4 \le v' \le 7$
MEL5	γ, a_1–a_8, v'	$\langle 5 \mid x^l \mid v'\rangle$, $0 \le l \le 8$, $5 \le v' \le 7$
MEL6	γ, a_1–a_8, v'	$\langle 6 \mid x^l \mid v'\rangle$, $0 \le l \le 8$, $6 \le v' \le 7$
MEL7	γ, a_1–a_8, v'	$\langle 7 \mid x^l \mid 7\rangle$, $0 \le l \le 8$
MELDV	γ, a_1–a_8, v, Δv	$\langle v \mid x^l \mid v + \Delta v\rangle$, $0 \le l \le 7$
ROTDEP	γ, a_1–a_8, J	$\gamma(\beta)$, $a_1(\beta)$–$a_8(\beta)$

Note that if $J \neq 0$ then all the quantities $\langle v \mid x^l \mid v'\rangle$ above become $\langle vJ \mid x^l \mid v'J\rangle$.

Table 3
Description of COMMON variables and arrays

Variable or array name	Description	
G	expansion parameter	γ
A1	potential energy coefficient	a_1
A2	potential energy coefficient	a_2
A3	potential energy coefficient	a_3
A4	potential energy coefficient	a_4
A5	potential energy coefficient	a_5
A6	potential energy coefficient	a_6
A7	potential energy coefficient	a_7
A8	potential energy coefficient	a_8
MEL (V, L, VP)	matrix element	$\langle v \mid x^l \mid v'\rangle$
V	vibrational quantum number	v
L	power of the reduced displacement x	l
VP	vibrational quantum number	v'
R (L, DV)	matrix element	$\langle v \mid x^l \mid v + \Delta v\rangle$
L	power of the reduced displacement x	l
DV	difference of vibrational quantum numbers	Δv

Table 4
Description of input parameters; the sample values of input parameters produce the results in the test-run output

Parameter name	Data format	Parameter description	Default value	Input required for IFLAG			Sample input parameters
				0	1	2	
TITLE	CHARACTER*80	heading, for information only		+	+	+	MOLECULE IS HCL ···
G	free	expansion parameter γ		+	+	+	0.007083694
A1	free	potential energy coefficient a_1		+	+	+	−2.3633725
A2	free	potential energy coefficient a_2		+	+	+	3.6605756
A3	free	potential energy coefficient a_3		+	+	+	−4.74921
A4	free	potential energy coefficient a_4		+	+	+	5.4529
A5	free	potential energy coefficient a_5		+	+	+	−5.5160
A6	free	potential energy coefficient a_6		+	+	+	4.2840
A7	free	potential energy coefficient a_7		+	+	+	−1.7260
A8	free	potential energy coefficient a_8		+	+	+	−0.0267
IFLAG	NAMELIST	program option IFLAG = 0 calculates $\langle v \mid x^l \mid v' \rangle$, $v = 0,\ldots,7$; $v \leqslant v' \leqslant 7$ 1 calculates $\langle v \mid x^l \mid v + \Delta v \rangle$ 2 calculates $\langle v \mid x^l \mid v' \rangle$, $v = 0,\ldots,7$; $v \leqslant v' \leqslant 7$ and $\langle v \mid x^l \mid v + \Delta v \rangle$					IFLAG = 2
JM	NAMELIST	maximum value of J	0	+	+	+	JM = 10
JINC	NAMELIST	increment for J	1	+	+	+	JINC = 10
VM	NAMELIST	maximum value of v' for $\langle v \mid x^l \mid v' \rangle$, VM $\leqslant 7$	7	+		+	VM = 5
VI	NAMELIST	initial value of v for $\langle v \mid x^l \mid v + \Delta v \rangle$			+	+	VI = 0
VIM	NAMELIST	maximum value of v for $\langle v \mid x^l \mid v + \Delta v \rangle$			+	+	VIM = 10
VINC	NAMELIST	incremental value of v for $\langle v \mid x^l \mid v + \Delta v \rangle$	1		+	+	VINC = 5
DVI	NAMELIST	initial value of Δv for $\langle v \mid x^l \mid v + \Delta v \rangle$			+	+	DVI = 0
DVF	NAMELIST	final value of Δv for $\langle v \mid x^l \mid v + \Delta v \rangle$			+	+	DVF = 5
DVINC	NAMELIST	incremental value of Δv for $\langle v \mid x^l \mid v + \Delta v \rangle$	1		+	+	

second group in which the v-dependence appears as a parameter to be set, it is important to recognize that for values of v greater than some value (that has to be determined empirically in each particular application) the series in powers of γ will fail to converge. For instance, the data in table 1 illustrate the values of the various contributions to $\langle v | x^3 | v+1 \rangle$ and $\langle v | x^2 | v+2 \rangle$ with $J = 0$ for a few values of v. From these results it is evident that acceptable convergence is attained at small values of v, for a given value of γ, but not at large values. For molecules with smaller values of γ than that of HCl, the convergence is correspondingly improved.

The test run for which the given main routine is furnished with the subroutines uses input data appropriate to HCl. This molecule has a value of $\gamma \approx 7 \times 10^{-3}$, typical of many molecules for which this program is expected to be useful.

The expressions in these subroutines have already been used in applications for the determinations of the dipole-moment functions of HCl [9,10] and CO [8] and the Herman–Wallis coefficients of CO [11].

3. Program description

Written in the language FORTRAN-77, the program VIBMATEL comprises a MAIN routine and ten subroutines. In the routine MAIN, the input data are read, the results are printed and the subroutines are called as required. The functions of the subroutines are stated in table 2. The meanings of the common variables and arrays are explained in table 3. The input data are described in table 4.

References

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TEST RUN INPUT

```
'MOLECULE IS HCL - DATA FROM COXON AND HOGILVIE, 1982.'
7.0836940-03 -2.3633725 3.6605756 -4.74921 5.4529 -5.516 4.284 -1.726 -.0267
 $SPEC IFLAG=2,JM=10,JINC=10,VM=5,VI=0,VIM=10,VINC=5,DVI=0,DVF=5 $END
```

TEST RUN OUTPUT

VALUES OF PARAMETERS FOR J= 0

GAMMA= .7083694-002 A1=-2.3633725 A2= 3.6605756 A3=-4.74921 A4= 5.4529
A5=-5.5150 A6= 4.2840 A7=-1.7260 A8= -.0267

VALUES OF THE MATRIX ELEMENTS FOR J= 0

<V:X**L:V'>

V	V'	X**0	X**1	X**2	X**3	X**4	X**5	X**6	X**7	X**8
0	0	1.0	.1268953-001	.3795038-002	.1714129-003	.4520551-004	.3806785-005	.9419550-006	.1182788-006	.2878924-007
0	1	.0	.5997500-001	.2553479-002	.7473368-003	.6669558-004	.1636570-004	.2205613-005	.5254865-006	.9234916-007
0	2	.0	-.5991628-002	.4772084-002	.3778598-003	.1341758-003	.1844255-004	.4928807-005	.9051370-006	.2325902-006
0	3	.0	.1026954-002	-.1182576-002	.4119566-003	.4597117-004	.2263320-004	.4288950-005	.1329662-005	.3101113-006
0	4	.0	-.2354034-003	.3181827-003	-.1879967-003	.3439899-004	.3834710-005	.3473779-005	.8603076-006	.3227618-006
0	5	.0	.6539508-004	-.9708946-004	.7266863-004	-.2697137-004	.2615604-005	-.9475748-007	.4537857-006	.1426927-006
1	1	1.0	.3861589-001	.1251302-001	.1130019-002	.2873765-003	.4129420-004	.9695636-005	.1795518-005	.4349991-006
1	2	.0	.8550141-001	.7397495-002	.2417929-002	.3579641-003	.9259824-004	.1794705-004	.4558485-005	.1042028-005
1	3	.0	-.1047636-001	.7974118-002	.1094910-002	.4422771-003	.9053218-004	.2681242-004	.6523907-005	.1866969-005
1	4	.0	.2072218-002	-.2327614-002	.7149143-003	.1289999-003	.7447117-004	.1998793-004	.7027678-005	.2084068-005
1	5	.0	-.5306349-003	.7045759-003	-.3927870-003	.5333365-004	.8629297-005	.1089343-004	.3788343-005	.1641053-005
2	2	1.0	.6542751-001	.2301101-001	.3404860-002	.9333825-003	.1876456-003	.4935750-004	.1170250-004	.3179090-005
2	3	.0	.1055844+000	.1393773-001	.5065770-002	.1051150-002	.3103087-003	.7749866-004	.2247078-004	.6216633-005
2	4	.0	-.1497057-001	.1083764-001	.2173345-002	.9917397-003	.2696143-003	.9170055-004	.2755225-004	.9043180-005
2	5	.0	.3309345-002	-.3619890-002	.9518495-003	.2510572-003	.1697541-003	.5940190-004	.2410918-004	.8649635-005
3	3	1.0	.9321276-001	.3547136-001	.7108762-002	.2210136-002	.5652065-003	.1708403-003	.4886570-004	.1521090-004
3	4	.0	.1229570+000	.2203119-001	.8349192-002	.2344600-002	.7899884-003	.2392148-003	.7961387-004	.2566429-004
3	5	.0	-.1954906-001	.1338311-001	.3613557-002	.1850798-002	.6255129-003	.2433075-003	.8646453-004	.3246702-004
4	4	1.0	.1220724+000	.5013696-001	.1259977-001	.4408269-002	.1354811-002	.4675534-003	.1553471-003	.5517841-004
4	5	.0	.1386783+000	.3164503-001	.1396882-001	.4476796-002	.1705272-002	.6020336-003	.2278838-003	.8329704-004
5	5	1.0	.1521198+000	.6716610-001	.2023738-001	.7897394-002	.2812913-002	.1096075-002	.4117460-003	.1652128-003

<V:X**L:V+DV>

V	V+DV	X**0	X**1	X**2	X**3	X**4	X**5	X**6	X**7
0	0	1.0	.1268934-001	.3795027-002	.1714315-003	.4520462-004	.3805742-005	.9418665-006	.1181700-006
5	5	1.0	.1516307+000	.6695534-001	.1996792-001	.7801073-002	.2700820-002	.1059474-002	.3756957-003
10	10	1.0	.3186498+000	.1954038+000	.1009166+000	.6111638-001	.3193640-001	.2009579-001	.9723029-002
0	1	.0	.5997504-001	.2553354-002	.7473206-003	.6657516-004	.1636345-004	.2202803-005	.5251794-006
5	6	.0	.1532555+000	.4258288-001	.2054009-001	.7556644-002	.3226262-002	.1236735-002	.5319193-003
10	11	.0	.2177980+000	.1212779+000	.8595346-001	.5084014-001	.3386542-001	.1837464-001	.1252188-001
0	2	.0	-.5991350-002	.4772193-002	.3778778-003	.1341721-003	.1843326-004	.4927046-005	.9025231-006
5	7	.0	-.2392441-001	.1750103-001	.7599334-002	.4798134-002	.2203404-002	.1085278-002	.4708604-003
10	12	.0	-.5476219-001	.2033263-001	.2388525-001	.2388304-001	.1784516-001	.1375972-001	.8259259-002
0	3	.0	.1026343-002	-.1182674-002	.4120085-003	.4600442-004	.2264184-004	.4290492-005	.1329338-005
5	8	.0	.8085819-002	-.8129735-002	.9058674-003	.7680714-003	.3404096-003	.5165034-003	.3043109-003
10	13	.0	.1959890-001	-.1662273-001	-.3898235-002	.7836455-003	.3690885-002	.4531385-002	.4268101-002
0	4	.0	-.2348080-003	.3181827-003	-.1880908-003	.3440668-004	.3839323-005	.3481114-005	.8634692-006
5	9	.0	-.2692748-002	.3410043-002	-.1405309-002	-.1549929-003	-.6122535-004	.8227573-004	.9052082-004
10	14	.0	-.7750505-002	.9255589-002	-.1811897-002	-.1657137-002	-.1304635-002	-.2862799-003	.6562660-003
0	5	.0	.6507706-004	-.9688744-004	.7270531-004	-.2698201-004	.2615734-005	-.9987517-007	.4538650-006
5	10	.0	.1046455-002	-.1462324-002	.8983243-003	-.1340407-003	-.3044986-004	-.4945424-004	-.9752341-005
10	15	.0	.3658633-002	-.4786642-002	.2207050-002	.4912427-003	.2532179-004	-.4805986-003	-.3869707-003

VALUES OF PARAMETERS FOR J=10

GAMMA= .7164583-002 A1=-2.3550207 A2= 3.6397808 A3=-4.70888 A4= 5.4007
A5=-5.4932 A6= 4.3422 A7=-1.8216 A8= -.0267

VALUES OF THE MATRIX ELEMENTS FOR J=10

<V:X**L:V'>

V	V'	X**0	X**1	X**2	X**3	X**4	X**5	X**6	X**7	X**8
0	0	1.0	.1280721-001	.3840264-002	.1750337-003	.4630323-004	.3933449-005	.9768878-006	.1236901-006	.3023652-007
0	1	.0	.6032007-001	.2592299-002	.7610761-003	.6852663-004	.1688037-004	.2293960-005	.5490557-006	.9724471-007
0	2	.0	-.6048627-002	.4824791-002	.3857481-003	.1374814-003	.1906423-004	.5118374-005	.9475419-006	.2447874-006
0	3	.0	.1040033-002	-.1200429-002	.4182059-003	.4714881-004	.2332264-004	.4458723-005	.1389536-005	.3266796-006
0	4	.0	-.2392223-003	.3241380-003	-.1917685-003	.3497703-004	.3936295-005	.3593693-005	.8986534-006	.3391610-006
0	5	.0	.6669655-004	-.9925535-004	.7442314-004	-.2751752-004	.2651686-005	-.1048161-006	.4699068-006	.1494620-006
1	1	1.0	.3898344-001	.1267097-001	.1205698-002	.2948277-003	.4271776-004	.1007895-004	.1880916-005	.4582059-006
1	2	.0	.8600070-001	.7512521-002	.2464791-002	.3681040-003	.9568557-004	.1869286-004	.4774681-005	.1099472-005
1	3	.0	-.1057961-001	.9059589-002	.1117935-002	.4535972-003	.9366702-004	.2789448-004	.6840184-005	.1969623-005
1	4	.0	.2099753-002	-.2363162-002	.7244978-003	.1322049-003	.7676043-004	.2079338-004	.7356042-005	.2198742-005
1	5	.0	-.5395980-003	.7180834-003	-.4005292-003	.5438474-004	.8797594-005	.1125931-004	.3957307-005	.1726371-005
2	2	1.0	.8607041-001	.2331951-001	.3481564-002	.9590319-003	.1943620-003	.5141784-004	.1228128-004	.3357349-005
2	3	.0	.1062110+000	.1416013-001	.5169147-002	.1081950-002	.3211986-003	.8034009-004	.2358853-004	.6572231-005
2	4	.0	-.1512418-001	.1094891-001	.2219393-002	.1018046-002	.2792149-003	.9556130-004	.2893292-004	.9561231-005
2	5	.0	.3355794-002	-.3675945-002	.9619155-003	.2570066-003	.1750268-003	.6183781-004	.2527245-004	.9139037-005
3	3	1.0	.9416207-001	.3597615-001	.7274961-002	.2274247-002	.5862213-003	.1783239-003	.5137350-004	.1610145-004
3	4	.0	.1236997+000	.2239297-001	.9039117-002	.2415760-002	.8190598-003	.2499050-003	.8374672-004	.2718235-004
3	5	.0	-.1975902-001	.1351209-001	.3690693-002	.1901594-002	.6484320-003	.2539616-003	.9093569-004	.3439681-004
4	4	1.0	.1233660+000	.5086404-001	.1290601-001	.4542918-002	.1407108-002	.4889653-003	.1635962-003	.5853566-004
4	5	.0	.1395325+000	.3218128-001	.1423402-001	.4617628-002	.1770921-002	.6293724-003	.2401855-003	.8837380-004
5	5	1.0	.1556035+000	.6824443-001	.2074973-001	.8150985-002	.2925509-002	.1148398-002	.4342996-003	.1756180-003

<V:X**L:V+DV>

V	V+DV	X**0	X**1	X**2	X**3	X**4	X**5	X**6	X**7
0	0	1.0	.1280701-001	.3840252-002	.1750212-003	.4630226-004	.3932314-005	.9767906-006	.1235714-006
5	5	1.0	.1532663+000	.6801329-001	.2045933-001	.8046080-002	.2805122-002	.1108569-002	.3953371-003
10	10	1.0	.3227167+000	.1993263+000	.1037375+000	.6336514-001	.3328616-001	.2113240-001	.1026509-001
0	1	.0	.6032012-001	.2592162-002	.7610584-003	.6850440-004	.1687790-004	.2290909-005	.5487176-006
5	6	.0	.1542136+000	.4331240-001	.2101834-001	.7795201-002	.3352361-002	.1293300-002	.5606077-003
10	11	.0	.2193566+000	.1236339+000	.6836249-001	.5261948-001	.3536509-001	.1927723-001	.1325573-001
0	2	.0	-.6048299-002	.4824914-002	.3857655-003	.1374772-003	.1905393-004	.5116416-005	.9446872-006
5	7	.0	-.2925193-001	.1764297-001	.7763912-002	.4937383-002	.2286561-002	.1135003-002	.4955189-003
10	12	.0	-.5551053-001	.2026543-001	.2442204-001	.2467080-001	.1857702-001	.1445733-001	.8717769-002
0	3	.0	.1039933-002	-.1200514-002	.4182664-003	.4718467-004	.2332661-004	.4460241-005	.1389154-005
5	8	.0	.8208663-002	-.8258833-002	.8592605-003	.7825746-003	.8670200-003	.5386243-003	.3199970-003
10	13	.0	.1995341-001	-.1690315-001	-.4151154-002	.7458251-003	.3801972-002	.4738020-002	.4507172-002
0	4	.0	-.2385540-003	.3241192-003	-.1918643-003	.3498743-004	.3941803-005	.3601358-005	.9020640-006
5	9	.0	-.2742061-002	.3480588-002	-.1428756-002	-.1655726-003	-.6638952-004	.8385428-004	.9460428-004
10	14	.0	-.7909028-002	.9470865-002	-.1812722-002	-.1738205-002	-.1379470-002	-.3220410-003	.6850323-003
0	5	.0	.6635307-004	-.9903939-004	.7445425-004	-.2762805-004	.2652411-005	-.1101244-006	.4700826-006
5	10	.0	.1069596-002	-.1498319-002	.9199920-003	-.1338538-003	-.3202687-004	-.5224597-004	-.1089498-004
10	15	.0	.3748477-002	-.4917231-002	.2257427-002	.5305534-003	.2987748-004	-.5085755-003	-.4160618-003