Modified rotation transformation method for the calculation of repulsion integrals

Liu Jingjiang *, Liu Fengying ** and Wang Yi

Nankai University, 300071 Tianjin, P.R. China

Received 17 April 1996; revised 9 April 1997

A modified rotation transformation method for two electron repulsion integrals is introduced in this paper. The percentage of nonzero matrix needed to perform the calculation is less than 30 in this method.

0. Introduction

In the ab initio method the total computational speed depends on the speed of calculation of the electron repulsion integrals. Molecular integrals with GTO basis have been reviewed recently [3]. There are many developments about the recurrence relation technique. McMurchie and Davidson (MD) proposed a recursion relationship [7] and performed its implementation [8]. Dupuis, Rye and King (DRK) proposed the use of a numerical quadrature [2,6] and that advantage be taken of a recurrence relation [11]. There are many works in which recurrence relations are proposed; they can make the calculation of ER1 and its derivatives [4,5,9] easier. Another local coordinate system method has been proposed by Pople and Hehre (PH) [10] and this technique was incorporated into the Gaussian 70 program. In the calculation of H_2O_2, the PH method requires only one fifth of the computation time required by the MD and DRK method [4]. It is believed that the local system method is very efficient, but in the PH method, the direction of the axes depends on the position of Q but not P, which means that the rotation transition of the P side axes are performed only. Hence, a modified rotation transformation method for two electron repulsion integrals is introduced in this paper.

1. The matrix expressions of repulsion integrals

The formula for electron repulsion integrals with GTO basis is

* To whom correspondence should be addressed.

** Now working in The Computer Center of Tianjin Petro-Chemical Corporation.

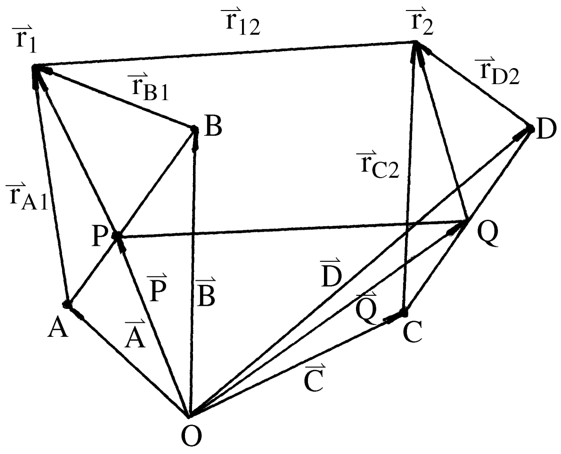

Figure 1. Relative position and vectors of points.

$$\mathrm{ER1}(1,2,3,4) = \int X_1(A, a_1, l_1, m_1, n_1) X_2(B, a_2, l_2, m_2, n_2) \times \frac{1}{r_{12}} X_3(C, a_3, l_3, m_3, n_3) X_4(D, a_4, l_4, m_4, n_4)\, \mathrm{d}\tau_1\, \mathrm{d}\tau_2. \quad (1.1)$$

In equation (1.1), X_1 and X_2 are functions of the first electron, the centers of X_1 and X_2 are on A and B, respectively, X_3 and X_4 are functions of the second electron, the centers of X_3 and X_4 are on C and D, respectively, as shown in figure 1.

According to the multiplication character of gaussian functions, we can transform two centers A and B into a single center P. Similarly, C and D can be transformed into Q. Then the four center repulsion integral equation (1.1) becomes a repulsion integral about the two centers P and Q expressed as follows:

$$\begin{aligned}\mathrm{ER1} = {} & N_1 N_2 N_3 N_4 \exp\left(-\frac{a_1 a_2}{a_1 + a_2}\overline{AB}^2\right) \exp\left(-\frac{a_3 a_4}{a_3 + a_4}\overline{CD}^2\right) \\ & \times \sum_{g_1 j_1 k_1} f_{g_1}\big(l_1, l_2, \overline{AP}_X, \overline{BP}_X\big) f_{j_1}\big(m_1, m_2, \overline{AP}_Y, \overline{BP}_Y\big) f_{k_1}\big(n_1, n_2, \overline{AP}_Z, \overline{BP}_Z\big) \\ & \times \sum_{g_2 j_2 k_2} f_{g_2}\big(l_3, l_4, \overline{CQ}_X, \overline{DQ}_X\big) f_{j_2}\big(m_3, m_4, \overline{CQ}_Y, \overline{DQ}_Y\big) f_{k_2}\big(n_3, n_4, \overline{CQ}_Z, \overline{DQ}_Z\big) \\ & \times \int X_P^{g_1} Y_P^{j_1} Z_P^{k_1} \exp\big(-\gamma_1 r_P^2\big) \frac{1}{r_{12}} X_Q^{g_2} Y_Q^{j_2} Z_Q^{k_2} \exp\big(-\gamma_2 r_Q^2\big)\, \mathrm{d}r_P\, \mathrm{d}r_Q. \quad (1.2)\end{aligned}$$

The constants f_{g_1}, f_{g_2}, f_{j_1}, f_{j_2}, f_{k_1} and f_{k_2} are the expansion coefficients used in transfering two centers to a single center, and N_i is the normalization coefficient of function i. The other symbols denote

$$\gamma_1 = a_1 + a_2, \quad (1.3)$$

Table 1
The ranks of suffix sets for orbitals up to d.

i	$g_1j_1k_1$	i	$g_1j_1k_1$	i	$g_1j_1k_1$	i	$g_1j_1k_1$
1	000	11	210	21	310	31	121
2	100	12	201	22	301	32	112
3	010	13	120	23	130	33	400
4	001	14	021	24	031	34	040
5	110	15	102	25	103	35	004
6	101	16	012	26	013		
7	011	17	111	27	022		
8	200	18	300	28	202		
9	020	19	030	29	022		
10	022	20	003	30	211		

$$\gamma_2 = a_3 + a_4, \tag{1.4}$$

$$\delta = 1/(4a_1) + 1/(4a_2), \tag{1.5}$$

where a_1, a_2, a_3 and a_4 are the exponential coefficients of functions X_1, X_2, X_3 and X_4, respectively. According to figure 1 we have

$$\vec{P} = \left(a_1 \vec{A} + a_2 \vec{B}\right)/\gamma_1, \tag{1.6}$$

$$\vec{Q} = \left(a_3 \vec{C} + a_4 \vec{D}\right)/\gamma_2, \tag{1.7}$$

$$\vec{AP} = \vec{P} - \vec{A} = \left(\vec{B} - \vec{A}\right)a_2/\gamma_1, \tag{1.8}$$

$$\vec{BP} = \vec{P} - \vec{B} = \left(\vec{A} - \vec{B}\right)a_1/\gamma_2, \tag{1.9}$$

$$\vec{CQ} = \vec{Q} - \vec{C} = \left(\vec{D} - \vec{C}\right)a_4/\gamma_2, \tag{1.10}$$

$$\vec{DQ} = \vec{Q} - \vec{D} = \left(\vec{C} - \vec{D}\right)a_3/\gamma_2. \tag{1.11}$$

In equation (1.2), $\overline{AB}$ denotes the distance between centers A and B, and $\overline{CD}$ denotes the distance between centers C and D. The suffix sets (g_1, j_1, k_1) and (g_2, j_2, k_2) are taken for combinations of all possible values. Suppose that there are n kinds of different combinations. If the orbitals up to d are considered, then n equals 35. The ranks of suffix sets are listed in table 1.

Let us use n-dimensional vectors to express the coefficient and coordinate sets:

$$F_P = \left[F_P^1, F_P^2, \ldots, F_P^n\right], \tag{1.12}$$

$$F_Q = \left[F_Q^1, F_Q^2, \ldots, F_Q^n\right], \tag{1.13}$$

$$X_P = \left[X_P^1, X_P^2, \ldots, X_P^n\right], \tag{1.14}$$

$$Y_Q = \left[Y_Q^1, Y_Q^2, \ldots, Y_Q^n\right], \tag{1.15}$$

where

$$F_P^i = f_{g_1}(l_1, l_2, \overline{AP}_X, \overline{BP}_X) f_{j_1}(m_1, m_2, \overline{AP}_Y, \overline{BP}_Y) f_{k_1}(n_1, n_2, \overline{AP}_Z, \overline{BP}_Z),$$
$$i = 1, \ldots, n, \tag{1.16}$$
$$F_Q^j = f_{g_2}(l_3, l_4, \overline{CQ}_X, \overline{DQ}_X) f_{j_2}(m_3, m_4, \overline{CQ}_Y, \overline{DQ}_Y) f_{k_2}(n_3, n_4, \overline{CQ}_Z, \overline{DQ}_Z),$$
$$j = 1, \ldots, n, \tag{1.17}$$
$$X_P^i = X_P^{g_1} Y_P^{j_1} Z_P^{k_1}, \quad i = 1, \ldots, n, \tag{1.18}$$
$$Y_Q^j = X_Q^{g_2} Y_Q^{j_2} Z_Q^{k_2}, \quad j = 1, \ldots, n. \tag{1.19}$$

The numerical orders of the suffix sets (g_1, j_1, k_1) and (g_2, j_2, k_2) correspond with the table 1 one to one.

Following equations (1.12)–(1.19), the formula (1.2) can be rewritten in matrix form as follows:

$$\mathrm{ER1} = N_1 N_2 N_3 N_4 \exp\left(-\frac{a_1 a_2}{a_1 + a_2} \overline{AB}^2\right) \exp\left(-\frac{a_3 a_4}{a_3 + a_4} \overline{CD}^2\right) F_P Z F_Q^{\mathrm{T}}. \tag{1.20}$$

In (1.20) Z is a $(n \times n)$ matrix defined as follows:

$$Z = X_P \widehat{Z} Y_Q^{\mathrm{T}}, \tag{1.21}$$

where Z is an operator and its effect is

$$X_P^i \widehat{Z} Y_P^j = \int X_P^i \exp(-\gamma_1 r_P^2) \frac{1}{r_{12}} Y_Q^j \exp(-\gamma_2 r_Q^2)\, \mathrm{d}r_P\, \mathrm{d}r_Q. \tag{1.22}$$

2. Application of the modified rotation transformation method in repulsion integrals

In the molecular system, let the points P and Q be the original points and their components in the directions of x, y and z be the basis vectors. These have two laboratory coordinate systems *AXES-P* and *AXES-Q*. They have parallel basis vectors as shown in figure 2. Take the same coordinate transformation for *AXES-P* and *AXES-Q* to make their components in the z direction overlap with $\overrightarrow{QP}$. This leads to the local coordinate systems *AXES-P'* and *AXES-Q'*, shown in figure 3.

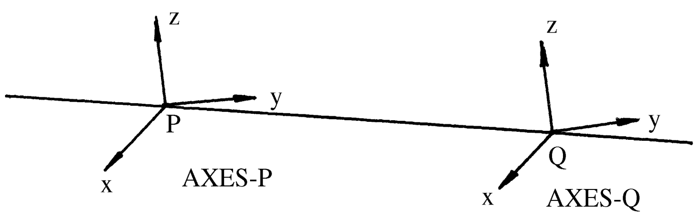

Figure 2. Laboratory coordinate system.

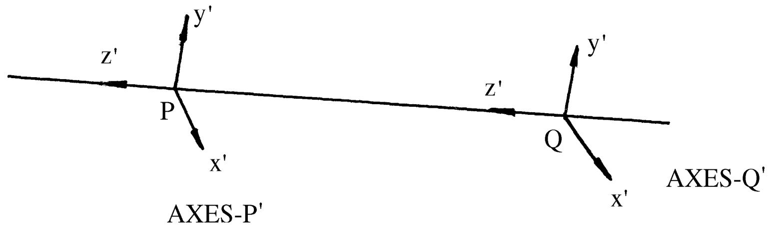

Figure 3. Local coordinate system.

Obviously, Euler rotation can transform the coordinate systems *AXES*-P and *AXES*-Q to *AXES*-P' and *AXES*-Q'. Let A be the transition matrix from *AXES*-P to *AXES*-P' or from *AXES*-Q to *AXES*-Q'. The relation is as follows:

$$\begin{bmatrix} X_P \\ Y_P \\ Z_P \end{bmatrix} = A \begin{bmatrix} X_{P'} \\ Y_{P'} \\ Z_{P'} \end{bmatrix}. \tag{2.1}$$

According to equation (2.1) we get a $(n \times n)$ matrix T. That is the transition matrix from $X_{P'}$ to X_P or from $Y_{Q'}$ to Y_Q:

$$X_P = TX_{P'} \quad \text{or} \quad Y_Q = TY_{Q'}, \tag{2.2}$$

$$T = \begin{bmatrix} t_{11} & t_{12} & \dots & t_{1n} \\ t_{21} & t_{22} & \dots & t_{2n} \\ \vdots & \vdots & \dots & \vdots \\ t_{n1} & t_{n2} & \dots & t_{nn} \end{bmatrix}. \tag{2.3}$$

Substituting formula (2.2) into (1.21) leads to the following relation:

$$Z = X_P \widehat{Z} Y_Q^{\mathrm{T}} = TX_{P'} \widehat{Z} Y_{Q'}^{\mathrm{T}} T^{\mathrm{T}} = TZ'T^{\mathrm{T}}, \tag{2.4}$$

where

$$Z' = X_{P'} \widehat{Z} Y_{Q'}^{\mathrm{T}}. \tag{2.5}$$

Because of the coordinate systems *AXES*-P' and *AXES*-Q' have the same z axes and x, y axes parallel to each other. There are many zero elements in the matrix Z' due to the "orthogonality of the orbitals". Because the two orbitals, centered on P and Q, respectively, have different symmetry (such as belonging to different irreducible representations of C_{2v} group), the integral between them should be zero [1]. When $n = 35$, there are 1225 elements in the Z' matrix, but only 335 of them are nonzero and all of the others are zero. For this reason, we first calculate all of the elements of matrix Z' according to formula (2.5), then, from equation (2.4), we can obtain the matrix Z of the original system.

3. The analytical expression of matrix Z'

The analytical expression of the two electron repulsion integrals is

$$\mathrm{ER1} = N_1 N_2 N_3 N_4 \exp\left(-\frac{a_1 a_2}{a_1 + a_2}\overline{AB}^2\right) \exp\left(-\frac{a_3 a_4}{a_3 + a_4}\overline{CD}^2\right)$$
$$\times \left[\sum_{g_1=0}^{l_1+l_2}\sum_{g_2=0}^{l_3+l_4}\sum_{j_1=0}^{m_1+m_2}\sum_{j_2=0}^{m_3+m_4}\sum_{k_1=0}^{n_1+n_2}\sum_{k_2=0}^{n_3+n_4} f_{g_1} f_{j_1} f_{k_1} f_{g_2} f_{j_2} f_{k_2}\right.$$
$$\left.\times \sum_{r_1,r_2,w}\sum_{g_1,g_2,v}\sum_{t_1,t_2,w} B_{r_1,r_2,u} B_{s_1,s_2,v} B_{t_1,t_2,w}\right] F_\nu\left(\frac{\overline{PQ}^2}{4\delta}\right), \tag{3.1}$$

where

$$F_m(\omega) = \int_0^1 \exp\left(-\omega t^2\right) t^{2m}\,\mathrm{d}t,$$
$$B_{r_1,r_2,u} = (-1)^{g_2} \frac{g_1! g_2!}{(4\beta_1)^{g_1}(4\beta_2)^{g_2}\delta^{g_1+g_2}} \frac{(4\beta_1)^{r_1}(4\beta_2)^{r_2}\delta^{2(r_1+r_2)}}{r_1! r_2! (g_1 - 2r_1)! (g_2 - 2r_2)!}$$
$$\times (g_1 + g_2 - 2r_1 - 2r_2)! \frac{(-1)^u \delta^u \overline{PQ}_x^{g_1+g_2-2u}}{u! [g_1 + g_2 - 2(r_1 + r_2) - 2u]!}, \tag{3.2}$$
$$\beta_1 = a_1 + a_2, \quad \beta_2 = a_3 + a_4, \quad \delta = \frac{1}{4\beta_1} + \frac{1}{4\beta_2},$$

and

$$\nu = g_1 + g_2 + j_1 + j_2 + k_1 + k_2 - (r_1 + r_2 + s_1 + s_2 + t_1 + t_2) - (u + v + w). \tag{3.3}$$

The cycling ranges of the suffixes $g_1,\ g_2,\ r_1,\ r_2$ and u are

$$g_1\colon\ 0 \sim l_1 + l_2; \quad g_2\colon\ 0 \sim l_3 + l_4; \quad r_1\colon\ 0 \sim \left[\frac{g_1}{2}\right]; \quad r_2\colon\ 0 \sim \left[\frac{g_2}{2}\right];$$
$$u\colon\ 0 \sim \left[\frac{g_1 + g_2 - 2(r_1 + r_2)}{2}\right].$$

The formulae for $B_{s_1,s_2,v}$ and $B_{t_1,t_2,w}$ have the similar form of $B_{r_1,r_2,u}$. They describe the components $\overline{PQ}y$ and $\overline{PQ}z$, respectively.

Comparing equation (3.1) with (1.7), we obtain the elements of matrix Z:

$$Z_{ij} = \sum_{r_1,r_2,u}\sum_{s_1,s_2,v}\sum_{t_1,t_2,w} B_{r_1,r_2,u} B_{s_1,s_2,v} B_{t_1,t_2,w} F_\nu\left(\frac{\overline{PQ}^2}{4\delta}\right). \tag{3.4}$$

The sets of suffices (g_1, j_1, k_1) and (g_2, j_2, k_2) correspond with the number sets in table 1.

When $n = 35$, there are 25 different kinds of combinations for the suffix set (g_1, g_2) as in table 2. For the same reason, the suffix sets (j_1, j_2) and (k_1, k_2) have

Table 2
Combinations for the suffix set (g_1, g_2).

g_1	g_2	g_1	g_2	g_1	g_2	g_1	g_2	g_1	g_2
0	0	0	2	0	3	3	3	4	2
1	0	2	1	3	1	4	0	2	4
0	1	1	2	1	3	0	4	4	3
1	1	2	2	3	2	4	1	3	4
2	0	3	0	2	3	1	4	4	4

25 different kinds of combinations, respectively. The form is the same for suffix set (g_1, g_2).

According to the combination forms of suffix set (g_1, g_2) in table 2, expand and calculate every term for $B_{r_1,r_2,u}$, and then merge the same-sort terms for ν following the definition the of ν in equation (3.3). Finally we obtain the expanding expressions of $B_{r_1,r_2,u}$ listed in table 3. Note that x is equal to the component $\overline{PQ}x$ that emerged in the formula (3.2).

On the basis of table 3 and according to the formula (3.4), we obtain the expression of each element of matrix Z'. In table 4 we listed the elements of matrix $Z'(35 \times 35)$. Its row indices vary with (g_1, j_1, k_1) and colument indices vary with (g_2, j_2, k_2). Note that all of the 335 nonzero elements are dependent only on $\overline{PQ}_Z$, but independent of $\overline{PQ}_X$ and $\overline{PQ}_Y$. The details are described in appendix B.

4. Conclusions

After the application of coordinate rotation transformation technology, due to the specialty of coordinate systems *AXES-*P' and *AXES-*Q', it is possible to construct the tables of elements for matrix Z'. Hence, the calculation of repulsion integrals involves arithmetic operations and matrix multiplications only. This method avoided the cycling of multiple suffixes. So we can say that the modified rotation transformation method for the computation of repulsion integrals is an improvement in program construction.

The program involving rotation transformation technology was run on an M340 computer. Comparing these results with those obtained from the method without this technology shows that the calculation speed was increased. In our program the percentage of nonzero matrix elements needed to perform the calculation is less than 30.

Appendix A

Table 3

g_1	g_2	C_{g_1,g_2}	$B_{\nu_1}(\nu_1 = g_1 + g_2 - 2r_1 - 2r_2 - u)$	
0	0	1	$B_1 = 1$	
1	0	$1/(4\beta_1\delta)$	$B_1 = x$	
0	1	$-1/(4\beta_2\delta)$	$B_1 = x$	
1	1	$-1/(4\beta_1 4\beta_2\delta^2)$	$B_1 = -2\delta$	$B_2 = x^2$
2	0	$\frac{2}{(4\beta_1\delta)^2}$	$B_0 = 4\beta_1\delta^2$ $B_2 = (1/2)x^2$	$B_1 = -\delta$
0	2	$\frac{2}{(4\beta_2\delta)^2}$	$B_0 = 4\beta_2\delta^2$ $B_2 = (1/2)x^2$	$B_1 = -\delta$
2	1	$\frac{-2}{(4\beta_1)^2 4\beta_2\delta^3}$	$B_1 = 4\beta_1\delta^2 x$ $B_3 = (1/2)x^3$	$B_2 = -3\delta x$
1	2	$\frac{2}{4\beta_1(4\beta_2)^2\delta^3}$	$B_1 = 4\beta_2\delta^2 x$ $B_3 = (1/2)x^3$	$B_2 = -3\delta x$
2	2	$\frac{4}{(4\beta_1 4\beta_2\delta^2)^2}$	$B_0 = 4\beta_1 4\beta_2\delta^4$ $B_2 = (1/2)\delta^2[x^2(4\beta_1 + 4\beta_2) + 6]$	$B_1 = -\delta^3(4\beta_1 + 4\beta_2)$ $B_3 = -3\delta x^2$ $B_4 = (1/4)x^4$
3	0	$\frac{6}{(4\beta_1\delta)^3}$	$B_1 = 4\beta_1\delta^2 x$ $B_3 = (1/6)x^3$	$B_2 = -\delta x$
0	3	$\frac{-6}{(4\beta_2\delta)^3}$	$B_1 = 4\beta_2\delta^2 x$ $B_3 = (1/6)x^3$	$B_2 = -\delta x$
3	1	$\frac{-6}{(4\beta_1)^3 4\beta_2\delta^4}$	$B_1 = -2\delta^3 4\beta_1$ $B_3 = -2\delta x^2$	$B_2 = \delta^2(2 + 4\beta_1 x^2)$ $B_4 = (1/6)x^4$

Table 3
(Continued.)

g_1 g_2	C_{g_1,g_2}	$B_{\nu_1}(\nu_1 = g_1 + g_2 - 2r_1 - 2r_2 - u)$	
1 3	$\frac{-6}{4\beta_1(4\beta_2)^3\delta^4}$	$B_1 = -2\delta^3 4\beta_2$ $B_3 = -2\delta x^2$	$B_2 = \delta^2(2 + 4\beta_2 x^2)$ $B_4 = (1/6)x^4$
3 2	$\frac{12}{(4\beta_1)^3(4\beta_2)^2\delta^5}$	$B_1 = 4\beta_1 4\beta_2 \delta^4 x$ $B_3 = (1/2)\delta^2 x[10 + x^2(4\beta_1 + (1/3)4\beta_2)]$ $B_5 = (1/12)x^5$	$B_2 = -\delta^3 x(3 \times 4\beta_1 + 4\beta_2)$ $B_4 = -(5/3)\delta x^3$
2 3	$\frac{-12}{(4\beta_1)^2(4\beta_2)^3\delta^5}$	$B_1 = 4\beta_1 4\beta_2 \delta^4 x$ $B_3 = (1/2)\delta^2 x[10 + x^2(4\beta_2 + (1/3)4\beta_1)]$ $B_5 = (1/12)x^5$	$B_2 = -\delta^3 x(4\beta_1 + 3 \times 4\beta_2)$ $B_4 = -(5/3)\delta x^3$
3 3	$\frac{-36}{(4\beta_1 4\beta_2 \delta^2)^3}$	$B_1 = -2\delta^5 4\beta_1 4\beta_2$ $B_3 = -2\delta^3[(5/3) + x^2(4\beta_1 + 4\beta_2)]$ $B_5 = -(5/6)\delta x^4$	$B_2 = -\delta^4[2(4\beta_1 + 4\beta_2) + 4\beta_1 4\beta_2 x^2]$ $B_4 = (1/6)\delta^2 x^2(30 + 4\beta_1 + 4\beta_2)$ $B_6 = (1/36)x^6$
4 0	$\frac{24}{(4\beta_1\delta)^4}$	$B_0 = (1/2)(4\beta_1\delta^2)^2$ $B_2 = (1/2)\delta^2(1 + 4\beta_1 x^2)$ $B_4 = (1/4!)x^4$	$B_1 = -4\beta_1\delta^3$ $B_3 = -(1/2)\delta x^2$
0 4	$\frac{24}{(4\beta_2\delta)^4}$	$B_0 = (1/2)(4\beta_2\delta^2)^2$ $B_2 = (1/2)\delta^2(1 + 4\beta_2 x^2)$ $B_4 = (1/4!)x^4$	$B_1 = -4\beta_2\delta^3$ $B_3 = -(1/2)\delta x^2$
4 1	$\frac{-24}{(4\beta_1)^4 4\beta_2\delta^5}$	$B_1 = (1/2)(4\beta_1\delta^2)^2 x$ $B_3 = (1/2)\delta^2 x(5 + 4\beta_1 x^2)$ $B_5 = (1/4!)x^5$	$B_2 = -3 \times 4\beta_1\delta^3 x$ $B_4 = -(5/6)\delta x^3$
1 4	$\frac{24}{4\beta_1(4\beta_2)^4\delta^5}$	$B_1 = (1/2)(4\beta_2\delta^2)^2 x$ $B_3 = (1/2)\delta^2 x(5 + 4\beta_2 x^2)$ $B_5 = (1/4!)x^5$	$B_2 = -3 \times 4\beta_2\delta^3 x$ $B_4 = -(5/6)\delta x^3$

Table 3
(Continued.)

g_1	g_2	C_{g_1,g_2}	$B_{\nu_1}(\nu_1 = g_1 + g_2 - 2r_1 - 2r_2 - u)$	
4	2	$\frac{48}{(4\beta_1)^4(4\beta_2)^2\delta^6}$	$B_0 = (1/2)(4\beta_1)^2 4\beta_2\delta^6$ $B_2 = (1/2)\delta^4[6\times 4\beta_1 + 4\beta_2 + 4\beta_1 x^2(2\beta_1 + 4\beta_2)]$ $B_4 = (1/4)\delta^2 x^4[15 + (4\beta_1 + (1/6)4\beta_2)x^2]$	$B_1 = -4\beta_1\delta^5(2\beta_1 + 4\beta_2)$ $B_3 = -(1/2)\delta^3[5 + x^2(6\times 4\beta_1 + 4\beta_2)]$ $B_5 = -(5/8)\delta x^4$ $B_6 = (1/48)x^6$
2	4	$\frac{48}{(4\beta_1)^2(4\beta_2)^4\delta^6}$	$B_0 = (1/2)4\beta_1(4\beta_2)^2\delta^6$ $B_2 = (1/2)\delta^4[6\times 4\beta_2 + 4\beta_1 + 4\beta_2 x^2(2\beta_2 + 4\beta_1)]$ $B_4 = (1/4)\delta^2 x^4[15 + (4\beta_2 + (1/6)4\beta_1)x^2]$	$B_1 = -4\beta_2\delta^5(4\beta_1 + 2\beta_2)$ $B_3 = -(1/2)\delta^3[5 + x^2(6\times 4\beta_2 + 4\beta_1)]$ $B_5 = -(5/8)\delta x^4$ $B_6 = (1/48)x^6$
4	3	$\frac{-4!3!}{(4\beta_1)^4(4\beta_2)^3\delta^7}$	$B_1 = (1/2)(4\beta_1)^2 4\beta_2\delta^6 x$ $B_3 = (1/2)\delta^4 x[10\times 4\beta_1 + 5\times 4\beta_2 + 4\beta_1 x^2((1/6)4\beta_1 + 4\beta_2)]$ $B_5 = (1/12)\delta^2 x^3[35 + (4\beta_1 + 2\beta_2)x^2]$	$B_2 = -(1/2)x\delta^5 4\beta_1(4\beta_1 + 6\times 4\beta_2)$ $B_4 = -(5/6)\delta^3 x[7 + x^2(2\times 4\beta_1 + 4\beta_2)]$ $B_6 = -(7/24)\delta x^5$ $B_7 = (1/144)x^7$
3	4	$\frac{4!3!}{(4\beta_1)^3(4\beta_2)^4\delta^7}$	$B_1 = (1/2)(4\beta_2)^2 4\beta_1\delta^6 x$ $B_3 = (1/2)\delta^4 x[10\times 4\beta_2 + 5\times 4\beta_1 + 4\beta_2 x^2((1/6)4\beta_2 + 4\beta_1)]$ $B_5 = (1/12)\delta^2 x^3[35 + x^2(2\beta_1 + 4\beta_2)]$	$B_2 = -(1/2)\delta^5 4\beta_2(4\beta_2 + 6\times 4\beta_1)x$ $B_4 = -(5/6)\delta^3 x[7 + x^2(2\times 4\beta_2 + 4\beta_1)]$ $B_6 = -(7/24)\delta x^5$ $B_7 = (1/144)x^7$
4	4	$\frac{(4!)^2}{(4\beta_1 4\beta_2\delta^2)^4}$	$B_0 = (1/4)(4\beta_1 4\beta_2\delta^4)^2$ $B_2 = (1/4)\delta^6[(4\beta_1)^2 + 12\times 4\beta_1 4\beta_2 + (4\beta_2)^2 + x^2 4\beta_1 4\beta_2(4\beta_1 + 4\beta_2)]$ $B_4 = (1/48)\delta^4\{x^4[(4\beta_1)^2 + (4\beta_2)^2 + 12\times 4\beta_1 4\beta_2] + 180x^2(4\beta_1$ $+ 4\beta_2) + 140\}$ $B_6 = (1/48)\delta^2 x^4[70 + (4\beta_1 + 4\beta_2)x^2]$	$B_1 = -(1/2)\delta^7 4\beta_1 4\beta_2(4\beta_1 + 4\beta_2)$ $B_3 = -(1/4)\delta^5\{10(4\beta_1 + 4\beta_2) + x^2[(4\beta_1 + 4\beta_2)^2$ $+ 10\times 4\beta_1 4\beta_2]\}$ $B_5 = -(5/24)\delta^3 x^2[28 + 3(4\beta_1 + 4\beta_2)x^2]$ $B_7 = -(7/72)\delta x^6$ $B_8 = (1/4!)^2 x^8$

Notes about table 3

(1) In table 3 we listed the expanding expressions of $B_{r_1,r_2,u}$. The decisions of symbols are as follow:

$$C_{g_1,g_2} = (-1)^{g_2} \frac{g_1!g_2!}{(4\beta_1)^{g_1}(4\beta_2)^{g_1}\delta^{g_1+g_2}}\,, \tag{A.1}$$

$$B_{\nu_1} = \frac{(4\beta_1)^{r_1}(4\beta_2)^{r_2}\delta^{2(r_1+r_2)}}{r_1!r_2!(g_1-2r_1)!(g_2-2r_2)!}(g_1+g_2-2r_1-2r_2)! \times \frac{(-1)^u\delta^u PQ_x^{g_1+g_2-2(r_1+r_2)-2u}}{u![g_1+g_2-2(r_1+2r_2)-2u]!}\,, \tag{A.2}$$

where

$$\nu_1 = g_1+g_2-2(r_1+r_2)-u. \tag{A.3}$$

Note that x in table 3 denotes component PQ_X emerged in equation (A.2).

(2) For a given value of suffix set (g_1, g_2), all expanding expressions of $B_{r_1',r_2',u}$ depend on the values of r_1, r_2 and u as are listed in table 3, and then, according to the definition of γ_1, merge the same-sort terms.

Appendix B

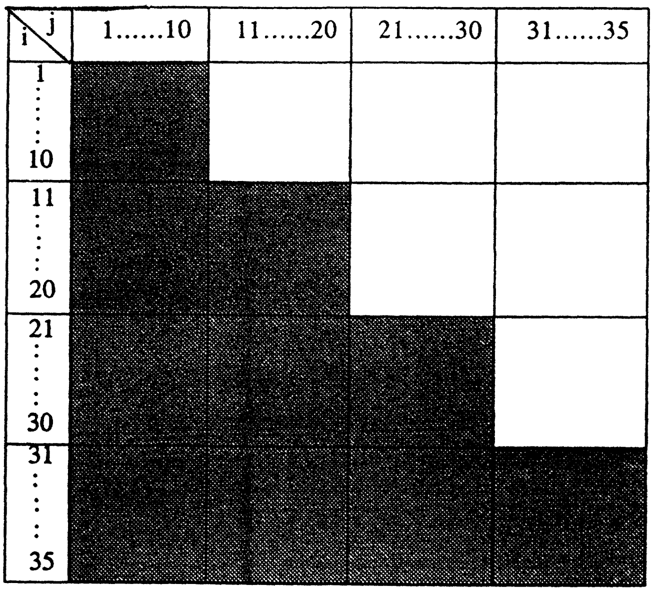

Figure 4.

Table 4

i	j	B_ν	i	j	B_ν	i	j	B_ν
1	1	1	10	4	$-2/[(4\beta_1)^2 4\beta_2\delta^3]$ $B_1 = 4\beta_1\delta^2 z$ $B_2 = -3\delta z$ $B_3 = (1/2)z^3$	19	3	$(18,2)$
1	4	$-1/4\beta_2\delta$ $B_1 = z$	11	3	$-2/[(4\beta_1)^3 4\beta_2\delta^4]$ $B_1 = -2\delta^3 4\beta_1$ $B_2 = 2\delta^2$	20	1	$6/(4\beta_1\delta)^3$ $B_1 = 4\beta_1\delta^2 x$ $B_2 = -\delta z$ $B_3 = (1/6)z^3$
2	2	$-1/(4\beta_1 4\beta_2\delta^2)$ $B_1 = -2\delta$	12	1	$2/(4\beta_1\delta)^3$ $B_1 = 4\beta_1\delta^2 z$ $B_2 = -\delta z$	20	4	$-6/[(4\beta_1)^3 4\beta_2\delta^4]$ $B_1 = -2\delta^3 4\beta_1$ $B_2 = \delta^2(2 + z^2 4\beta_1)$ $B_3 = -2\delta z^2$ $B_4 = (1/6)z^4$
3	3	$(2,2)$	12	4	$-2/[(4\beta_1)^3 4\beta_2\delta^4]$ $B_1 = -2\delta^3 4\beta_1$ $B_2 = \delta^2(z^2 4\beta_1 + 2)$ $B_3 = -\delta z^2$	22	2	$-6/[(4\beta_1)^4 4\beta_2\delta^5]$ $B_2 = -2\delta^3 z 4\beta_1$ $B_3 = 2\delta^2 z$
4	1	$1/4\beta_1\delta$ $B_1 = z$	13	2	$(11,3)$	24	3	$(22,2)$
4	4	$-1/(4\beta_1 4\beta_2\delta^2)$ $B_1 = -2\delta$ $B_2 = z^2$	14	1	$(12,1)$	25	2	$-6/[(4\beta_1)^4 4\beta_2\delta^5]$ $B_2 = -2\delta^3 z 4\beta_1$ $B_3 = 2\delta^2 z$ $B_4 = -(1/3)\delta z^3$
6	2	$-1/[(4\beta_1)^2 4\beta_2\delta^3]$ $B_2 = -2\delta z$	14	4	$(12,4)$	26	3	$(25,2)$
7	3	$(6,2)$	15	2	$(16,3)$	27	1	$4/(4\beta_1\delta)^4$ $B_0 = (4\beta_1)^2\delta^4$ $B_1 = -2\delta^3 4\beta_1$ $B_2 = \delta^2$
8	1	$2/(4\beta_1\delta)^2$ $B_0 = 4\beta_1\delta^2$ $B_1 = -\delta$	16	3	$-2/[(4\beta_1)^3 4\beta_2\delta^4]$ $B_1 = -2\delta^3 4\beta_1$ $B_2 = 2\delta^2$ $B_3 = -\delta z^2$			
8	4	$(9,4)$						
9	1	$(8,1)$						
9	4	$-2/[(4\beta_1)^2 4\beta_2\delta^3]$ $B_1 = 4\beta_1\delta^2 z$ $B_2 = -\delta z$						

Table 4
(Continued.)

i	j	B_ν
10	1	$2/(4\beta_1\delta^2)$ $B_0 = 4\beta_1\delta^2$ $B_1 = -\delta$ $B_2 = -(1/2)z^2$
28	1	$4/(4\beta_1\delta)^4$ $B_0 = \delta^4(4\beta_1)^2$ $B_1 = -2\delta^3 4\beta_1$ $B_2 = (1/2)\delta^2(2 + z^2 4\beta_1)$ $B_3 = -(1/2)\delta z^2$
28	4	$-4/[(4\beta_1)^4 4\beta_2\delta^5]$ $B_1 = \delta^4 z(4\beta_1)^2$ $B_2 = -4\delta^3 z 4\beta_1$ $B_3 = (1/2)\delta^2 z(6 + z^2 4\beta_1)$ $B_4 = -(1/2)\delta z^3$
29	1	$(28, 1)$
29	4	$(28, 4)$
30	3	$-2/[(4\beta_1)^4 4\beta_2\delta^5]$ $B_2 = -2\delta^3 z 4\beta_1$ $B_3 = -2\delta^2 z$

i	j	B_ν
18	2	$-6/[(4\beta_1)^3 4\beta_2\delta^4]$ $B_1 = -2\delta^3 4\beta_1$ $B_2 = 2\delta^2$
34	4	$(33, 4)$
35	1	$24/(4\beta_1\delta)^4$ $B_0 = (1/2)\delta^4(4\beta_1)^2$ $B_1 = -\delta^3 4\beta_1$ $B_2 = (1/2)\delta^2(1 + z^2 4\beta_1)$ $B_3 = -(1/2)\delta z^2$ $B_4 = (1/24)z^4$
35	4	$-24/[(4\beta_1)^2 4\beta_2\delta^5]$ $B_1 = (1/2)(4\beta_1)^2 z\delta^4$ $B_2 = -3\delta^3 z 4\beta_1$ $B_3 = (1/2)\delta^2 z(5 + z^2 4\beta_1)$ $B_4 = -(5/6)\delta z^3$ $B_5 = (1/24)z^5$
2	6	$1/[4\beta_1(4\beta_2)^2\delta^3]$ $B_2 = -2\delta z^2$
3	7	$(2, 6)$
5	5	$4/(4\beta_1 4\beta_2\delta^2)^2$ $B_2 = 4\delta^2$

i	j	B_ν
27	4	$-4/[(4\beta_1)^4 4\beta_2\delta^5]$ $B_1 = \delta^4 z(4\beta_1)^2$ $B_2 = -2\delta^3 z(4\beta_1)$ $B_3 = \delta^2 z$
15	6	$2/[(4\beta_1)^3(4\beta_2)^2\delta^5]$ $B_2 = -2\delta^3 z^4 4\beta_1$ $B_3 = 6\delta^2 z$ $B_4 = -\delta z_3$
16	7	$(15, 6)$
17	5	$1/[(4\beta_1)^3(4\beta_2)^2\delta^5]$ $B_3 = 4\delta^2 z$
18	6	$6/[(4\beta_1)^3(4\beta_2)^2\delta^5]$ $B_2 = -2\delta^3 z 4\beta_1$ $B_3 = 2\delta^2 z$
19	7	$(18, 6)$
21	5	$6/[(4\beta_1)^4(4\beta_2)^2\delta^6]$ $B_2 = 4\delta^4 4\beta_1$ $B_3 = -4\delta^3$
22	6	$6/[(4\beta_1)^4(4\beta_2)^2\delta^6]$ $B_2 = 4\delta^2 4\beta_1$ $B_3 = -2\delta^3(2 + z^2 4\beta_1)$ $B_4 = 2\delta^2 z^2$

Table 4
(Continued.)

i	j	B_ν	i	j	B_ν	i	j	B_ν
31	2	$(30,3)$	6	6	$1/(4\beta_1 4\beta_2\delta^2)^2$	23	5	$(21,5)$
33	1	$24/(4\beta_1\delta)^4$				24	7	$(22,6)$
					$B_2 = 4\delta^2$	26	7	$(25,6)$
		$B_0 = (1/2)\delta^4(4\beta_1)^2$			$B_3 = -2\delta z^2$	30	7	$(31,6)$
		$B_1 = -\delta^3 4\beta_1$						
		$B_2 = (1/2)\delta^2$						
33	4	$-24/[(4\beta_1)^4 4\beta_2\delta^5]$	7	7	$(6,6)$	25	6	$6/[(4\beta_1)^4(4\beta_2)^2\delta^6]$
			11	7	$2/[(4\beta_1)^3(4\beta_2)^2\delta^5]$			
		$B_1 = (1/2)(4\beta_1)^2 z\delta^4$						$B_2 = 4\delta^4 4\beta_1$
		$B_2 = -4\beta_1\delta^3 z$			$B_2 = -2\delta^3 z 4\beta_1$			$B_3 = -2\delta^3(2 + z^2 4\beta_1)$
		$B_3 = (1/2)\delta^2 z$			$B_3 = 2\delta^3 z$			$B_4 = 4\delta^2 z^2$
34	1	$(33,1)$	13	6	$(11,7)$			$B_5 = -(1/3)\delta z^4$
31	6	$2/[(4\beta_1)^4(4\beta_2)^2\delta^6]$	8	10	$4/(4\beta_1 4\beta_2\delta^2)^2$	12	10	$4/[(4\beta_1)^3(4\beta_2)^2\delta^5]$
		$B_2 = 4\delta^4 4\beta_1$			$B_0 = 4\beta_1 4\beta_2\delta^4$			$B_1 = 4\beta_1 4\beta_2\delta^4 z$
		$B_3 = -2\delta^3(2 + z^2 4\beta_1)$			$B_1 = -\delta^3(4\beta_1 + 4\beta_2)$			$B_2 = -\delta^3 z(3 \times 4\beta_1 + 4\beta_2)$
		$B_4 = 2\delta^2 z^2$			$B_2 = (1/2)\delta^2(2 + z^2 4\beta_1)$			$B_3 = (1/2)\delta^3 z(6 + z^2 4\beta_1)$
					$B_3 = -(1/2)\delta z^2$			$B_4 = -(1/2)\delta z^3$
32	5	$2/[(4\beta_1)^4(4\beta_2)^2\delta^6]$	9	8	$4/(4\beta_1 4\beta_2\delta^2)^2$	14	8	$(12,9)$
						14	9	$(12,8)$
		$B_2 = 4\delta^4 4\beta_1$			$B_0 = 4\beta_1 4\beta_2\delta^4$	14	10	$(12,10)$
		$B_3 = -4\delta^3$			$B_1 = -\delta^3(4\beta_1 + 4\beta_2)$			
		$B_4 = 2\delta^2 z^2$			$B_2 = \delta^2$			

Table 4
(Continued.)

i	j	B_ν
1	8	$2/(4\beta_2\delta)^2$ $B_0 = 4\delta_2\delta^2$ $B_1 = -\delta$
1	9	$(1,8)$
1	10	$2/(4\beta_2\delta^2)^2$ $B_0 = 4\beta_2\delta^2$ $B_1 = -\delta$ $B_2 = (1/2)z^2$
4	8	$2/[4\beta_1(4\beta_2)^2\delta^3]$ $B_1 = \delta^2 z 4\beta_2$ $B_3 = -\delta z$
4	9	$(4,8)$
4	10	$2/[4\beta_1(4\beta_2)^2\delta^3]$ $B_1 = \delta^2 z 4\beta_2$ $B_2 = -3\delta z$ $B_4 = (1/2)z$

i	j	B_ν
9	9	$(8,8)$
9	10	$(8,10)$
10	8	$4/(4\beta_1\beta_2\delta^2)^2$ $B_0 = 4\beta_1 4\beta_2\delta^4$ $B_1 = -\delta^3(4\beta_1 + 4\beta_2)$ $B_2 = (1/2)\delta^2(2 + z^2 4\beta_2)$ $B_3 = -(1/2)\delta z^2$
10	9	$(10,8)$
10	10	$4/(4\beta_1 4\beta_2\delta^2)^2$ $B_0 = 4\beta_1 4\beta_2\delta^4$ $B_1 = -\delta^3(4\beta_1 + 4\beta_2)$ $B_2 = (1/2)\delta^2[6 + z^2(4\beta_1 + 4\beta_2)]$ $B_3 = -3\delta z^2$ $B_4 = (1/4)z^4$
12	8	$4/[(4\beta_1)^3(4\beta_2)^2\beta^5]$ $B_1 = 4\beta_1 4\beta_2\delta^4 z$ $B_2 = -\delta^3 z(4\beta_1 + 4\beta_2)$ $B_3 = 3\delta^2 z$

i	j	B_ν
20	8	$12/[(4\beta_1)^3(4\beta_2)^2\delta^5]$ $B_1 = \delta^4 z 4\beta_1 4\beta_2$ $B_2 = -\delta^3 z(4\beta_1 + 4\beta_2)$ $B_3 = \delta^2 z[1 + (1/6)z^2 4\beta_2]$ $B_4 = -(1/6)\delta z^3$
20	9	$(20,8)$
20	10	$12/[(4\beta_1)^3(4\beta_2)^2\delta^5]$ $B_1 = \delta^4 z^4 4\beta_1 4\beta_2$ $B_2 = -\delta^3 z(3\times 4\beta_1 + 4\beta_2)$ $B_3 = (1/6)\delta^2 z[30 + (3\times 4\beta_1$ $+ 4\beta_2)z^2]$ $B_4 = -(5/3)\delta z^3$ $B_5 = (1/2)z^5$
27	8	$8/[(4\beta_1)^4(4\beta_2)^2\delta^6]$ $B_0 = (4\beta_1)^2 4\beta_2\delta^6$ $B_1 = -\delta^5 4\beta_1(4\beta_1 + 2\times 4\beta_2)$ $B_2 = \delta^4(4\times 4\beta_1 + 4\beta_2)$ $B_3 = -3\delta^3$

Table 4
(Continued.)

i	j	B_ν	i	j	B_ν	i	j	B_ν
8	8	$4/(4\beta_1 4\beta_2 \delta^2)^2$ $B_0 = 4\beta_1 4\beta_2 \delta^4$ $B_1 = -\delta^3(4\beta_1 + 4\beta_2)$ $B_2 = 3\delta^2$	12	9	$4/[(4\beta_1)^3(4\beta_2)^2\delta^5]$ $B_1 = 4\beta_1 4\beta_2 \delta^4 z$ $B_2 = -\delta^3 z(4\beta_1 + 4\beta_2)$ $B_3 = \delta^2 z$	27	9	$(27, 8)$
8	9	$(9, 8)$				27	10	$8/[(4\beta_1)^4(4\beta_2)^2\delta^6]$ $B_0 = (4\beta_1)^2 4\beta_2 \delta^6$ $B_1 = -\delta^5 4\beta_1(4\beta_1 + 2 \times 4\beta_2)$ $B_2 = (1/2)\delta^4[z^2(4\beta_1)^2 + 4 \times 4\beta_1$ $+ 2 \times 4\beta_2]$ $B_3 = -\delta^3(1 + z^2 4\beta_1)$ $B_4 = (1/2)\delta^2 z^2$
28	8	$8/[(4\beta_1)^4(4\beta_2)^2\delta^6]$ $B_0 = (4\beta_1)^2 4\beta_2 \delta^6$ $B_1 = -\delta^5 4\beta_1(4\beta_1 + 2 \times 4\beta_2)$ $B_2 = \delta^4[4 \times 4\beta_1 + 4\beta_2$ $+ z^2(1/2)4\beta_1 4\beta_2]$ $B_3 = -(1/2)\delta^3[6 + z^2(4\beta_1 + 4\beta_2)]$ $B_4 = (3/2)\delta^2 z^2$	33	9	$48/[(4\beta_1)^2\delta^6(4\beta_2)^2]$ $B_0 = (1/2)(4\beta_1)^2 4\beta_2 \delta^6$ $B_1 = -(1/2)\delta^5 4\beta_1(4\beta_1 + 2 \times 4\beta_2)$ $B_2 = \delta^4(4\beta_1 + 2\beta_2)$ $B_3 = -(1/2)\delta^3$	35	10	$48/[(4\beta_1)^4(4\beta_2)^2\delta^6]$ $B_0 = (1/2)(4\beta_1)^2 4\beta_2 \delta^6$ $B_1 = -(1/2)\delta^5 4\beta_1(2 \times 4\beta_2 + 4\beta_1)$ $B_2 = (1/2)\delta^4[6 \times 4\beta_1 + 4\beta_2$ $+ (1/2)z^2 4\beta_1(4\beta_1$ $+ 2 \times 4\beta_2)]$ $B_3 = -(1/2)\delta^3[5 + (6 \times 4\beta_1$ $+ 4\beta_2)z^2]$ $B_4 = (1/4)\delta^2 z^2[15 + (4\beta_1$ $+ (1/6)4\beta_2)z^2]$ $B_5 = -(5/8)\delta z^4$ $B_6 = (1/48)z^6$
28	9	$8/[(4\beta_1)^4(4\beta_2)^2\delta^6]$ $B_0 = (4\beta_1)^2 4\beta_2 \delta^6$ $B_1 = -\delta^5 4\beta_1(4\beta_1 + 2 \times 4\beta_2)$ $B_2 = \delta^4[2 \times 4\beta_1 + 4\beta_2$ $+ z^2(1/2)4\beta_1 4\beta_2 \delta^4]$ $B_3 = -(1/2)\delta^3[2 + z^2(4\beta_1 + 4\beta_2)]$ $B_4 = (1/2)\delta^2 z^2$	33	10	$48/[(4\beta_1)^4(4\beta_2)^2\delta^6]$ $B_0 = (1/2)(4\beta_1)^2 4\beta_2 \delta^6$ $B_1 = -(1/2)\delta^5 4\beta_1(4\beta_1 + 2 \times 4\beta_2)$ $B_2 = (1/4)\delta^4[4 \times 4\beta_1 + 8\beta_2$ $+ z^2(4\beta_2)^2]$ $B_3 = -(1/2)\delta^3(1 + z^2 4\beta_1)$ $B_4 = (1/4)\delta^2 z^2$			

Table 4
(Continued.)

i	j	B_ν
28	10	$8/[(4\beta_1)^4(4\beta_2)^2\delta^6]$ $B_0=(4\beta_1)^2 4\beta_2\delta^6$ $B_1=-\delta^5 4\beta_1(4\beta_1+2\times 4\beta_2)$ $B_2=(1/2)\delta^4[z^2 4\beta_1(4\beta_1+4\beta_2)$ $+2(4\times 4\beta_1+4\beta_2)]$ $B_3=-(1/2)\delta^3[6+z^2(4\beta_2$ $+7\times 4\beta_1)]$ $B_4=(1/4)\delta^2 z^2(12+z^2 4\beta_1)$ $B_5=-(1/4)\delta z^4$
29	8	$(28, 9)$
29	9	$(28, 8)$
29	10	$(28, 10)$
15	13	$-4/(4\beta_1 4\beta_2\delta^2)^3$ $B_1=-2\delta^5 4\beta_1 4\beta_2$ $B_2=2\delta^4(4\beta_1+4\beta_2)$ $B_3=-\delta^3(2+z^2 4\beta_2)$ $B_4=\delta^2 z^2$
18	13	$(11, 19)$
19	11	$(18, 13)$
20	12	$-4/(4\beta_1 4\beta_2\delta^2)^3$ $B_1=-2\delta^5 4\beta_1 4\beta_2$ $B_2=\delta^4[2(4\beta_1+4\beta_2)+z^2 4\beta_1 4\beta_2]$ $B_3=-\delta^3[2+z^2(4\beta_1+4\beta_2\times 2)]$ $B_4=(1/6)\delta^2 z^2(12+z^2 4\beta_2)$ $B_5=-(1/6)\delta z^4$

i	j	B_ν
34	8	$(33, 9)$
34	9	$(33, 8)$
34	10	$(33, 10)$
12	12	$-4/(4\beta_1 4\beta_2\delta^2)^3$ $B_1=-2\delta^5 4\beta_1 4\beta_2$ $B_2=2\delta^4(4\beta_1+4\beta_2+4\beta_1 4\beta_2 z^2)$ $B_3=-\delta^3[6+(4\beta_1+4\beta_2)z^2]$ $B_4=3\delta^2 z^2$
35	8	$48/[(4\beta_1)^4(4\beta_2)^2\delta^6]$ $B_0=(1/2)(4\beta_1)^2 4\beta_2\delta^6$ $B_1=-(1/2)\delta^5 4\beta_1(4\beta_1+2\times 4\beta_2)$ $B_2=(1/2)\delta^4[2\times 4\beta_1+4\beta_2$ $+z^4 4\beta_1 4\beta_2]$ $B_3=-(1/2)\delta^3(1+z^2 4\beta_1+4\beta_2)$ $B_4=(1/24)\delta^2 z^2(12+4\beta_2 z^2)$ $B_5=-(1/24)\delta z^4$
35	9	$(35, 8)$
28	12	$-8/[(4\beta_1)^4(4\beta_2)^3\delta^7]$ $B_1=\delta^6 z(4\beta_1)^2 4\beta_2$ $B_2=-\delta^5 z 4\beta_1(4\times 4\beta_2+4\beta_1)$ $B_3=(1/2)\delta^4 z[6(2\times 4\beta_1$ $+4\beta_2)+z^2 4\beta_1 4\beta_2]$ $B_4=-(1/2)\delta^3 z[18+z^2(4\beta_1+4\beta_2)]$ $B_5=(3/2)\delta^2 z^3$

i	j	B_ν
11	11	$-4/[(4\beta_1 4\beta_2\delta^2)^3]$ $B_1=-2\delta^5 4\beta_1 4\beta_2$ $B_2=2\delta^4(4\beta_1+4\beta_2)$ $B_3=-6\delta^3$
13	13	$(11, 11)$
14	12	$(12, 14)$
33	8	$48/[(4\beta_1)^4(4\beta_2)^2\delta^6]$ $B_0=(1/2)(4\beta_1)^2 4\beta_2\delta^6$ $B_1=-(1/2)\delta^5 4\beta_1(4\beta_1+2\times 4\beta_2)$ $B_2=(1/2)\delta^4(6\times 4\beta_1+4\beta_2)$ $B_3=-(5/2)\delta^3$
16	11	$(15, 13)$
35	12	$-48/[(4\beta_1)^4(4\beta_2)^3\delta^7]$ $B_1=(1/2)\delta^6 z(4\beta_1)^2 4\beta_2$ $B_2=-(1/2)\delta^5 z 4\beta_1(4\beta_1+6\times 4\beta_2)$ $B_3=(1/2)\delta^4 z(6\times 4\beta_1+5\times 4\beta_2$ $+z^2 4\beta_1 4\beta_2)$ $B_4=-(1/6)\delta^3 z^3(3\times 4\beta_1+5\times 4\beta_2$ $+(5/2)\delta^3 z)$ $B_5=(1/24)\delta^2 z^3(20+4\beta_2 z^2)$ $B_6=-(1/24)\delta z^5$

Table 4
(Continued.)

i	j	B_ν	i	j	B_ν	i	j	B_ν
22	13	$-12/[(4\beta_1)^4(4\beta_2)^3\delta^7]$ $B_2 = -2\delta^5 4\beta_1 4\beta_2$ $B_3 = 2\delta^4(4\beta_1 + 4\beta_2)$ $B_4 = -2\delta^3 z$	30	11	$-4/[(4\beta_1)^4(4\beta_2)^3\delta^7]$ $B_2 = -2\delta^5 z 4\beta_1 4\beta_2$ $B_3 = 2\delta^4 z(4\beta_1 + 4\beta_2)$ $B_4 = -6\delta^3 z$	11	16	$-4/(4\beta_1 4\beta_2\delta^2)^3$ $B_1 = -2\delta^5 4\beta_1 4\beta_2$ $B_2 = 2\delta^4(4\beta_1 + 4\beta_2)$ $B_3 = -\delta^3(2 + z^2 4\beta_1)$ $B_4 = \delta^2 z^2$
24	11	(22, 13)	31	11	(30, 11)			
25	13	$-12/[(4\beta_1)^4(4\beta_2)^3\delta^7]$ $B_2 = -2z\delta^5 4\beta_1 4\beta_2$ $B_3 = 2\delta^4(4\beta_1 + 4\beta_2)z$ $B_4 = -(1/3)\delta^3 z(6 + z^2 4\beta_2)$ $B_5 = (1/3)\delta^2 z^3$	33	12	$-48/[(4\beta_1)^4(4\beta_2)^3\delta^7]$ $B_1 = (1/2)z\delta^6(4\beta_1)^2 4\beta_2$ $B_2 = -(1/2)\delta^5 z 4\beta_1(4\beta_1 + 2 \times 4\beta_2)$ $B_3 = (1/2)\delta^4 z(6 \times 4\beta_1 + 4\beta_2)$ $B_4 = -(5/2)\delta^3 z$	12	14	$-4/(4\beta_1 4\beta_2\delta^2)^3$ $B_1 = -2\delta^5 4\beta_1 4\beta_2$ $B_2 = \delta^4[2(4\beta_1 + 4\beta_2) + z^2 4\beta_1\beta_2]$ $B_3 = -\delta^3[2 + (2\beta_1 + 4\beta_2)z^2]$ $B_4 = \delta^2 z^2$
26	11	(25, 13)	34	12	(33, 14)	13	15	(11, 16)
27	12	$-8/[(4\beta_1)^4(4\beta_2)^3\delta^7]$ $B_1 = \delta^6 z(4\beta_1)^2 4\beta_2$ $B_2 = -\delta^5 z 4\beta_1(2 \times 4\beta_2 + 4\beta_1)$ $B_3 = \delta^4(4 \times 4\beta_1 + 4\beta_2)z$ $B_4 = -3\delta^3 z$						
29	12	(28, 14)	14	14	(12, 12)	29	12	(28, 14)
15	15	$-4/(4\beta_1 4\beta_2\delta^2)^3$ $B_1 = -2\delta^5 4\beta_1 4\beta_2$ $B_2 = 2\delta^4(4\beta_1 + 4\beta_2)$ $B_3 = -\delta^3[6 + (4\beta_1 + 4\beta_2)z^2]$ $B_4 = 6\delta^2 z^2$ $B_5 = -(1/2)\delta z^4$	25	15	$-12/[(4\beta_1)^4(4\beta_2)^3\delta^7]$ $B_2 = -2\delta^5 z 4\beta_1 4\beta_2$ $B_3 = 2\delta^4 z(3 \times 4\beta_1 + 4\beta_2)$ $B_4 = -(1/3)\delta^3 z[30 + z^2(3 \times 4\beta_1 + 4\beta_2)]$ $B_5 = (10/3)\delta^2 z^3$ $B_6 = -(1/6)\delta z^5$	32	17	$-2/[(4\beta_1)^4(4\beta_2)^3\delta^7]$ $B_3 = 4z\delta^4 4\beta_1$ $B_4 = -12\delta^3 z$ $B_5 = 2\delta^2 z^3$

Table 4
(Continued.)

i	j	B_ν	i	j	B_ν	i	j	B_ν
16	16	$(15, 15)$	26	26	$(25, 15)$	33	14	$-48/[(4\beta_1)^4(4\beta_2)^2\delta^7]$ $B_1 = (1/2)\delta^6 z(4\beta_1)^2 4\beta_2$ $B_2 = -(1/2)z\delta^5 4\beta_1(4\beta_1 + 2 \times 4\beta_2)$ $B_3 = (1/2)\delta^4 z(2 \times 4\beta_1 + 4\beta_2)$ $B_4 = -(1/2)\delta^3 z$
17	17	$-1/(4\beta_1 4\beta_2\delta^2)^3$ $B_3 = -8\delta^3$ $B_4 = 4\delta^2 z^2$	27	14	$(27, 12)$			
			28	14	$-8/[(4\beta_1)^4(4\beta_2)^3\delta^7]$ $B_1 = \delta^6 z(4\beta_1)^2 4\beta_2$ $B_2 = -\delta^5 z 4\beta_1(4\beta_1 + 4 \times 4\beta_2)$ $B_3 = (1/2)\delta^4 z[2(4 \times 4\beta_1 + 3 \times 4\beta_2)$ $+ z^2 4\beta_1 4\beta_2]$ $B_4 = -(1/2)\delta^3 z[6 + (4\beta_1 + 4\beta_2)z^2]$ $B_5 = (1/2)\delta^2 z^3$			
18	15	$-4/(4\beta_1 4\beta_2\delta^2)^3$ $B_1 = -2\delta^5 4\beta_1 4\beta_2$ $B_2 = 2\delta^4(4\beta_1 + 4\beta_2)$ $B_3 = -\delta^3(2 + z^2 4\beta_1)$ $B_4 = \delta^2 z^2$						
19	16	$(18, 15)$				34	14	$(33, 12)$
20	14	$(20, 12)$	29	14	$(28, 12)$	35	14	$(35, 12)$
21	17	$-6/[(4\beta_1)^4(4\beta_2)^3\delta^7]$ $B_3 = 4\delta^4 z 4\beta_1$ $B_4 = -4\delta^3 z$	30	16	$-4/[(4\beta_1)^4(4\beta_2)^3\delta^7]$ $B_2 = -2\delta^5 z 4\beta_1 4\beta_2$ $B_3 = 2\delta^4 z(3 \times 4\beta_1 + 4\beta_2)$ $B_4 = -\delta^2 z(6 + z^2 4\beta_1)$ $B_5 = \delta^2 z^2$	11	19	$-12/[(4\beta_1 4\beta_2\delta^2)^3]$ $B_1 = -2\delta^5 4\beta_1 4\beta_2$ $B_2 = 2\delta^4(4\beta_1 + 4\beta_2)$ $B_3 = -2\delta^3$
22	15	$-12/[(4\beta_1)^4(4\beta_2)^3\delta^7]$ $B_2 = -2\delta^5 4\beta_1 4\beta_2$ $B_3 = 2\delta^4 z(3 \times 4\beta_1 + 4\beta_2)$ $B_4 = -\delta^2 z(6 + z^2 4\beta_1)$ $B_5 = \delta^2 z^3$				12	20	$-12/(4\beta_1 4\beta_2\delta^2)^3$ $B_1 = -2\delta^5 4\beta_1 4\beta_2$ $B_2 = \delta^4[2(4\beta_1 + 4\beta_2)z^2 4\beta_1 4\beta_2]$ $B_3 = -\delta^3[2 + (2 \times 4\beta_1 + 4\beta_2)z^2]$ $B_4 = (1/6)\delta^5 z^2(12 + z^2 4\beta_1)$ $B_5 = -(1/6)\delta z^3$

Table 4
(Continued.)

i	j	B_ν
23	17	$(21, 17)$
24	16	$(22, 15)$
15	18	$-12/(4\beta_1 4\beta_2 \delta^2)^3$ $B_1 = -2\delta^5 4\beta_1 4\beta_2$ $B_2 = 2\delta^4(4\beta_1 + 4\beta_2)$ $B_3 = -\delta^3(2 + z^2 4\beta_2)$ $B_4 = \delta^2 z^2$
16	19	$(15, 18)$
18	18	$-36/(4\beta_1 4\beta_2 \delta^2)^3$ $B_1 = -2\delta^5 4\beta_1 4\beta_2$ $B_2 = 2\delta^4(4\beta_1 + 4\beta_2)$ $B_4 = -(10/3)\delta^3$
19	19	$(18, 18)$
20	20	$-36/(4\beta_1 4\beta_2 \delta^2)^3$ $B_1 = -2\delta^5 4\beta_1 4\beta_2$ $B_2 = \delta^4[2(4\beta_1 + 4\beta_2) + z^2 4\beta_1 4\beta_2]$ $B_3 = -(1/3)\delta^3[10 + 6(4\beta_1 + 4\beta_2)z^2]$ $B_4 = (1/6)\delta^2 z^2[30 + (4\beta_1 + 4\beta_2)]$ $B_5 = -(5/6)\delta z^4$ $B_6 = -(1/36)z^6$

i	j	B_ν
31	15	$(30, 16)$
27	20	$-24/[(4\beta_1)^4(4\beta_2)^3\delta^7]$ $B_1 = \delta^6 z(4\beta_1)^2 4\beta_2$ $B_2 = -\delta^5 z 4\beta_1(4\beta_1 + 2 \times 4\beta_2)$ $B_3 = (1/6)\delta^4 z[6(2 \times 4\beta_1 + 4\beta_2)$ $+ z^2(4\beta_1)^2]$ $B_4 = -(1/3)\delta^3 z(3 + z^2 4\beta_1)$ $B_5 = (1/6)\delta z^3$
28	20	$-24/[(4\beta_1)^4(4\beta_2)^3\delta^7]$ $B_1 = \delta^6 z(4\beta_1)^2 4\beta_2$ $B_2 = -\delta^5 z 4\beta_1(4\beta_1 + 4 \times 4\beta_2)$ $B_3 = (1/6)\delta^4 z[18(2 \times 4\beta_1 + 4\beta_2)$ $+ z^2 4\beta_1(4\beta_1 + 3 \times 4\beta_2)]$ $B_4 = -(1/6)\delta^3 z[30 + z^2(11 \times 4\beta_1$ $+ 3 \times 4\beta_2)]$ $B_5 = (1/12)\delta^2 z^3(20 + 4\beta_1 z^2)$ $B_6 = -(1/12)\delta z^5$

i	j	B_ν
13	8	$(11, 19)$
14	20	$(12, 20)$
34	20	$(33, 20)$
35	20	$-144/[(4\beta_1)^4(4\beta_2)^3\delta^7]$ $B_1 = (1/2)\delta^6 z(4\beta_1)^2 4\beta_2$ $B_2 = -(1/2)\delta^5 z 4\beta_1(4\beta_1 + 6 \times 4\beta_2)$ $B_3 = (1/12)\delta^4 z[30(2 \times 4\beta_1 + 4\beta_2)$ $+ z^2 4\beta_1(4\beta_1 + 6 \times 4\beta_2)]$ $B_4 = -(5/6)\delta^3 z[7 + (2 \times 4\beta_1$ $+ 4\beta_2)z^2]$ $B_5 = (1/12)\delta^2 z^2[35 + (4\beta_1$ $+ 4\beta_2)z^2]$ $B_6 = -(7/24)\delta z^5$ $B_7 = (1/144)z^7$
21	21	$36/(4\beta_1 4\beta_2 \delta^2)^4$ $B_2 = 4\delta^6 4\beta_1 4\beta_2$ $B_3 = -4\delta^5(4\beta_1 + 4\beta_2)$ $B_4 = (20/3)\delta^4$
21	23	$36/(4\beta_1 4\beta_2 \delta^2)^4$ $B_2 = 4\delta^6 4\beta_1 4\beta_2$ $B_3 = -4\delta^5(4\beta_1 + 4\beta_2)$ $B_4 = 4\delta^4$

Table 4
(Continued.)

i	j	B_ν
22	18	$-36/[(4\beta_1)^4(4\beta_2)^3\delta^7]$ $B_2 = -2\delta^5 z^4 4\beta_1 4\beta_2$ $B_3 = 2\delta^4 z(4\beta_1 + 4\beta_2)$ $B_4 = -(10/3)\delta^3 z$
24	19	$(22, 18)$
25	18	$-36/[(4\beta_1)^4(4\beta_2)^3\delta^7]$ $B_2 = -2\delta^5 z 4\beta_1 4\beta_2$ $B_3 = 2\delta^4 z(4\beta_1 + 4\beta_2)$ $B_4 = -(1/3)\delta^3 z(6 + z^2 4\beta_2)$
26	19	$(25, 18)$
25	22	$36/(4\beta_1 4\beta_2 \delta^2)^4$ $B_2 = 4\delta^6 4\beta_1 4\beta_2$ $B_3 = -2\delta^5[2(4\beta_1 + 4\beta_2)$ $\quad + z^2 4\beta_1 4\beta_2]$ $B_4 = 4\delta^4 + 2\delta^4 z^4(4\beta_1 + 2 \times 4\beta_2)$ $B_5 = -(1/3)\delta^3 z^2(z^2 4\beta_2 + 12)$ $B_6 = (1/3)\delta^2 z^4$

i	j	B_ν
29	20	$(28, 20)$
30	19	$-12/[(4\beta_1)^4(4\beta_2)^3\delta^7]$ $B_2 = -2\delta^5 z 4\beta_1 4\beta_2$ $B_3 = 2\delta^4 z(4\beta_1 + 4\beta_2)$ $B_4 = -2\delta^3 z$
33	20	$-144/[(4\beta_1)^4(4\beta_2)^3\delta^7]$ $B_1 = (1/2)\delta^5 z(4\beta_1)^2 4\beta_2$ $B_2 = -(1/2)\delta^5 z 4\beta_1(4\beta_1 + 2 \times 4\beta_2)$ $B_3 = (1/12)\delta^4 z[6(4\beta_1 + 4\beta_2)$ $\quad + z^2(4\beta_1)^2]$ $B_4 = -(1/6)\delta^3 z(3 + z^2 4\beta_1)$ $B_5 = (1/12)\delta^2 z^3$
26	24	$(25, 22)$
26	26	$(25, 25)$
30	24	$12/(4\beta_1 4\beta_2 \delta^2)^4$ $B_2 = 4\delta^6 4\beta_1 4\beta_2$ $B_3 = -2\delta^5[2(4\beta_1 + 4\beta_2)$ $\quad + z^2 4\beta_1 4\beta_2]$ $B_4 = 2\delta^4[2 + z^2(4\beta_1 + 4\beta_2)]$ $B_5 = -2\delta^3 z^2$

i	j	B_ν
22	22	$36/(4\beta_1 4\beta_2 \delta^2)^4$ $B_2 = 4\delta^6 4\beta_1 4\beta_2$ $B_3 = -2\delta^5[2(4\beta_1 + 4\beta_2)$ $\quad + z^2 4\beta_1 4\beta_2]$ $B_4 = (1/3)\delta^4[20 + 6z^2(4\beta_1 4\beta_2)]$ $B_5 = -(10/3)\delta^3 z^2$
23	21	$(21, 23)$
23	23	$(21, 21)$
27	29	$16/(4\beta_1 4\beta_2 \delta^2)^4$ $B_0 = (4\beta_1 4\beta_2 \delta^4)^2$ $B_1 = -2\delta^7 4\beta_1 4\beta_2(4\beta_1 + 4\beta_2)$ $B_2 = (1/2)\delta^6[(8 \times 4\beta_1 4\beta_2$ $\quad + 2(4\beta_1 + 4\beta_2)^2 + z^2 4\beta_2(4\beta_1)^2]$ $B_3 = -(1/2)\delta^5\{z^2[(4\beta_1)^2 + 2$ $\quad \times 4\beta_1\beta_2] + 8(4\beta_1 + 4\beta_2)\}$ $B_4 = (1/2)\delta^4[6 + z^2(4 \times 4\beta_1 + 4\beta_2)]$ $B_5 = -(3/2)\delta^3 z^2$

Table 4
(Continued.)

i	j	B_ν
31	22	$(30, 24)$
32	21	$12/(4\beta_1 4\beta_2 \delta^2)^4$ $B_2 = 4\delta^6 4\beta_1 4\beta_2$ $B_3 = -4\delta^5(4\beta_1 + 4\beta_2)$ $B_4 = 2\delta^4[2 + z4\beta_2]$ $B_5 = -2\delta^3 z^2$
32	23	$(32, 21)$
22	25	$36/(4\beta_1 4\beta_2 \delta^2)^4$ $B_2 = 4\delta^6 4\beta_1 4\beta_2$ $B_3 = -2\delta^5[2(2 \times 4\beta_1 + 4\beta_2)$ $+ z^2 4\beta_1 4\beta_2]$ $B_4 = 4\delta^4 + 2\delta^4 z^2(4\beta_2 + 2 \times 4\beta_1)$ $B_5 = -(1/3)\delta^3 z^2 + (12 + 4\beta_1 z^2)$ $B_6 = (1/3)\delta^2 z^4$
22	24	$(22, 22)$
24	26	$(22, 25)$
30	26	$12/(4\beta_1 4\beta_2 \delta^2)^4$ $B_2 = 4\delta^6 4\beta_1 4\beta_2$ $B_3 = -2\delta^5[2(4\beta_1 + 4\beta_2) + z^2 4\beta_1 4\beta_2]$ $B_4 = 2\delta^4[2 + z^2(2 \times 4\beta_1 + 4\beta_2)]$ $B_5 = -(1/3)\delta^3 z^2(12 + 4\beta_1 z^2)$ $B_6 = -(1/3)\delta^2 z^4$
31	25	$(30, 26)$
27	27	$16/(4\beta_1 4\beta_2 \delta^2)^4$ $B_0 = (4\beta_1 4\beta_2 \delta^2)^4$ $B_1 = -2\delta^7 4\beta_1 4\beta_2(4\beta_1 + 4\beta_2)$ $B_2 = \delta^2[(4\beta_1 + 4\beta_2)^2 + 6 \times 4\beta_1 4\beta_2]$ $B_3 = -6\delta^5(4\beta_1 + 4\beta_2)$ $B_4 = 9\delta^4$
29	27	$16/(4\beta_1 4\beta_2 \delta^2)^4$ $B_0 = (4\beta_1 4\beta_2 \delta^4)^2$ $B_1 = -2\delta^7 4\beta_1 4\beta_2(4\beta_1 + 4\beta_2)$ $B_2 = (1/2)\delta^6\{[8 \times 4\beta_1 4\beta_2 + 2(4\beta_1$ $+ 4\beta_2)^2] + z^2 4\beta_1(4\beta_2)^2]\}$ $B_3 = -(1/2)\delta^5[z^2(2 \times 4\beta_1$ $+ 4\beta_2)4\beta_2 + 8(4\beta_1 + 4\beta_2)]$ $B_4 = (1/2)\delta^4[6 + z^2(2 \times 4\beta_2 + 4\beta_1)]$ $B_5 = -(3/2)\delta^3 z^2$

Table 4
(Continued.)

i	j	B_ν	i	j	B_ν	i	j	B_ν
25	25	$36/(4\beta_1 4\beta_2 \delta^2)^4$ $B_2 = 4\delta^6 4\beta_1 4\beta_2$ $B_3 = -2\delta^5[2(4\beta_1 + 4\beta_2) + z^2 4\beta_1 4\beta_2]$ $B_4 = (1/3)\delta^4[20 + 12z^2(4\beta_1 + 4\beta_2)]$ $B_5 = -(1/3)\delta^3 z^2(30 + 4\beta_1 + 4\beta_2)$ $B_6 = (5/3)\delta^2 z^4$ $B_7 = -(1/18)\delta z^6$	27	28	$(27, 29)$	29	29	$16/(4\beta_1 4\beta_2 \delta^2)^4$ $B_0 = (4\beta_1 4\beta_2 \delta^4)^2$ $B_1 = -2\delta^7 4\beta_1 4\beta_2(4\beta_1 + 4\beta_2)$ $B_2 = (1/2)\delta^6\{2[6 \times 4\beta_1 4\beta_2 + (4\beta_1 + 4\beta_2)^2] + 4\beta_1 z^4 4\beta_2(4\beta_1 + 4\beta_2)\}$ $B_3 = -(1/2)\delta^5\{(4\beta_1 + 4\beta_2)12 + z^2[(4\beta_1 + 4\beta_2)^2 + 12 \times 4\beta_1 4\beta_2]\}$ $B_4 = (1/4)\delta^4\{36 + z^2[18(4\beta_1 + 4\beta_2) + z^2 4\beta_1 4\beta_2]\}$ $B_5 = -(1/4)\delta^3 z^2[36 + (4\beta_1 + 4\beta_2)z^2]$ $B_6 = (3/4)\delta^2 z^4$
			28	27	$(29, 27)$			
			28	28	$(29, 29)$			
			28	29	$(29, 28)$			
29	28	$16/(4\beta_1 4\beta_2 \delta^2)^4$ $B_0 = (4\beta_1 4\beta_2 \delta^4)^2$ $B_1 = -2\delta^7 4\beta_1 4\beta_2(4\beta_1 + 4\beta_2)$ $B_2 = (1/2)\delta^6\{2[4 \times 4\beta_1 4\beta_2 + (4\beta_1 + 4\beta_2)^2] + 4\beta_1 z^2 4\beta_2(4\beta_1 + 4\beta_2)\}$ $B_3 = -(1/2)\delta^5\{(4\beta_1 + 4\beta_2)8 + z^2[(4\beta_1 + 4\beta_2)^2 + 6 \times 4\beta_1 4\beta_2]\}$ $B_4 = (1/4)\delta^4\{12 + z^2[14(4\beta_1 + 4\beta_2) + z^2 4\beta_1 4\beta_2]\}$ $B_5 = -(1/4)\delta^3 z^2[12 + (4\beta_1 + 4\beta_2)z^2]$ $B_6 = (1/4)\delta^2 z^4$	33	29	$96/(4\beta_1 4\beta_2 \delta^2)^4$ $B_0 = (1/2)(4\beta_1 4\beta_2 \delta^4)^2$ $B_1 = -\delta^7 4\beta_1 4\beta_2(4\beta_1 + 4\beta_2)$ $B_2 = (1/4)\delta^6 2[2 \times 4\beta_1 4\beta_2 + (4\beta_1 + 4\beta_2)^2] + 4\beta_2(4\beta_1)^2 z^2\}$ $B_3 = -(1/4)\delta^5[4(4\beta_1 + 4\beta_2) + z^2 4\beta_1(4\beta_1 + 2 \times 4\beta_2)]$ $B_4 = (1/4)\delta^4[2 + z^2(2 \times 4\beta_1 + 4\beta_2)^2]$ $B_5 = -(1/4)\delta^3 z^2$	35	29	$96/(4\beta_1 4\beta_2 \delta^2)^4$ $B_0 = (1/2)(4\beta_1 4\beta_2 \delta^4)^2$ $B_1 = -\delta^7 4\beta_1 4\beta_2(4\beta_1 + 4\beta_2)$ $B_2 = (1/2)\delta^6[(4\beta_1 + 4\beta_2)^2 + 6 \times 4\beta_1 4\beta_2 + z^2 4\beta_1(4\beta_1 + 2 \times 4\beta_2)]$ $B_3 = -(1/4)\delta^5\{(4\beta_1 + 4\beta_2)12 + z^2[(4\beta_1)^2 + 14 \times 4\beta_1 4\beta_2 + 2(4\beta_2)^2]\}$ $B_4 = (1/4)\delta^4[10 + (12 \times 4\beta_1 + 17 \times 4\beta_2)z^2 + (1/48)z^4 4\beta_2 \times (3 \times 4\beta_1 + 32 \times 4\beta_2)]$ $B_5 = -(1/12)\delta^3 z^2[45 + z^2(3 \times 4\beta_1 + 8 \times 4\beta_2)]$
			34	27	$(33, 27)$			
			34	28	$(33, 29)$			

Table 4
(Continued.)

i	j	B_ν	i	j	B_ν	i	j	B_ν
								$B_6 = (1/48)\delta^2 z^4(30 + 4\beta_2 z^2)$ $B_7 = -(1/48)\delta z^6$
33	27	$96/(4\beta_1 4\beta_2 \delta^2)^4$ $B_0 = (1/2)(4\beta_1 4\beta_2 \delta^4)^2$ $B_1 = -\delta^7 4\beta_1 4\beta_2(4\beta_1 + 4\beta_2)$ $B_2 = (1/2)\delta^6[(4\beta_1 + 4\beta_2)^2$ $+ 6 \times 4\beta_1 4\beta_2]$ $B_3 = -3\delta^5(4\beta_1 + 4\beta_2)$ $B_4 = (5/2)\delta^4$	34	29	$(33, 28)$	30	30	$4/(4\beta_1 4\beta_2 \delta^2)^4$ $B_2 = 4\delta^6 4\beta_1 4\beta_2$ $B_3 = -2\delta^5[2(4\beta_1 + 4\beta_2)$ $+ z^2 4\beta_1 4\beta_2]$ $B_4 = 2\delta^4[6 + z^2(4\beta_1 + 4\beta_2)]$ $B_5 = -6\delta^3 z$
			35	27	$96/(4\beta_1 4\beta_2 \delta^2)^4$ $B_0 = (1/2)(4\beta_1 4\beta_2 \delta^4)^2$ $B_1 = -\delta^7 4\beta_1 4\beta_2(4\beta_1 + 4\beta_2)$ $B_2 = (1/2)\delta^6[(4\beta_1 + 4\beta_2) + 2$ $\times 4\beta_1 4\beta_2] + z^2 4\beta_1(4\beta_2)^2$ $B_3 = -(1/2)\delta^5[2(4\beta_1 + 4\beta_2)$ $+ z^2 4\beta_2(2 \times 4\beta_1 + 4\beta_2)]$ $B_4 = (1/24)\delta^4\{12[1 + (4\beta_1 + 2$ $\times 4\beta_2)z^2] + z^2(4\beta_2)^2\}$ $B_5 = -(1/12)\delta^3 z^2(6 + 4\beta_2 z^2)$ $B_6 = (1/24)\delta^2 z^2$	31	31	$(30, 30)$
33	28	$96/(4\beta_1 4\beta_2 \delta^2)^4$ $B_0 = (1/2)(4\beta_1 4\beta_2 \delta^4)^2$ $B_1 = -\delta^7 4\beta_1 4\beta_2(4\beta_1 + 4\beta_2)$ $B_2 = (1/4)\delta^6\{2[(4\beta_1 + 4\beta_2)^2 + 6$ $\times 4\beta_1 4\beta_2] + 4\beta_2(4\beta_1)^2 z^2\}$ $B_3 = -(1/4)\delta^5[(4\beta_1 + 4\beta_2)12$ $+ z^2 4\beta_1(4\beta_1 + 2 \times 4\beta_2)]$ $B_4 = (1/4)\delta^4[10 + z^2(6 \times 4\beta_1$ $+ 4\beta_2)]$ $B_5 = -(5/4)\delta^3 z^2$				32	32	$4/(4\beta_1 4\beta_2 \delta^2)^4$ $B_2 = 4\delta^6 4\beta_1 4\beta_2$ $B_3 = -4\delta^5(4\beta_1 + 4\beta_2)$ $B_4 = 2\delta^4[6 + z^2(4\beta_1 + 4\beta_2)]$ $B_5 = -12\delta^3 z^2$ $B_6 = \delta^2 z^4$
			35	28	$(35, 27)$			

Table 4
(Continued.)

i	j	B_ν	i	j	B_ν
33	33	$(4!)^2/(4\beta_1 4\beta_2 \delta^2)^4$ $B_0 = 0.25(\delta^4 4\beta_1 4\beta_2)^2$ $B_1 = -0.5\delta^7 4\beta_1 4\beta_2(4\beta_1 + 4\beta_2)$ $B_2 = 0.25\delta^6[(4\beta_1)^2 + 12 \times 4\beta_1 4\beta_2 + (4\beta_2)^2]$ $B_3 = -2.5\delta^5(4\beta_1 + 4\beta_2)$	35	33	$(4!)^2/(4\beta_1 4\beta_2 \delta^2)^4$ $B_0 = 0.25(\delta^4 4\beta_1 4\beta_2)^2$ $B_1 = -0.5\delta^7 4\beta_1 4\beta_2(4\beta_1 + 4\beta_2)$ $B_2 = (1/4)\delta^6[(4\beta_1)^2 + 4 \times 4\beta_1 4\beta_2 + (4\beta_2)^2 + z^2 4\beta_1(4\beta_2)^2]$ $B_3 = -(1/4)\delta^5\{2(4\beta_1 + 4\beta_2) + z^2[(4\beta_2)^2 + 2 \times 4\beta_1 4\beta_2]\}$ $B_4 = (1/4)\delta^4\{1 + z^2[4\beta_1 + 2 \times 4\beta_2 + (1/12)z^2(4\beta_2)^2]\}$ $B_5 = (1/48)\delta^2 z^4$
33	34	$(4!)^2/(4\beta_1 4\beta_2 \delta^2)^4$ $B_0 = 0.25(\delta^4 4\beta_1 4\beta_2)^2$ $B_1 = -0.5\delta^7 4\beta_1 4\beta_2(4\beta_1 + 4\beta_2)$ $B_2 = 0.25\delta^6[4 \times 4\beta_1 4\beta_2 + (4\beta_1)^2 + (4\beta_2)^2]$ $B_3 = -0.5\delta^5(4\beta_1 + 4\beta_2)$ $B_4 = 0.25\delta^4$			
33	35	$(4!)^2/(4\beta_1 4\beta_2 \delta^2)^4$ $B_0 = 0.25(\delta^4 4\beta_1 4\beta_2)^2$ $B_1 = -0.5\delta^7 4\beta_1 4\beta_2(4\beta_1 + 4\beta_2)$ $B_2 = (1/4)\delta^6[(4\beta_1)^2 + 4 \times 4\beta_1 4\beta_2 + (4\beta_1)^2]$ $+ 0.25\delta^6 z^2 4\beta_2(4\beta_1)^2$ $B_3 = -(1/2)\delta^5(4\beta_1 + 4\beta_2) - 0.25\delta^5 z^2$ $\times [(4\beta_1)^2 + 2 \times 4\beta_1\beta_2]$ $B_4 = (1/4)\delta^4[1 + z^2(2 \times 4\beta_1 + 4\beta_2)$ $+ (1/12)(z4\beta_1)^2]$ $B_5 = -(1/48)\delta^3 z^2(12 + 4\beta_1 z^2)$ $B_6 = (1/48)\delta^2 z^4$	35	35	$(4!)^2/(4\beta_1 4\beta_2 \delta^2)^4$ $B_0 = 0.25(\delta^4 4\beta_1 4\beta_2)^4$ $B_1 = -0.5\delta^7 4\beta_1 4\beta_2(4\beta_1 + 4\beta_2)$ $B_2 = (1/4)\delta^6[(4\beta_1)^2 + 12 \times 4\beta_1 4\beta_2 + (4\beta_2)^2]$ $+ (1/4)\delta^6 z^2 4\beta_1 4\beta_2(4\beta_1 + 4\beta_2)$ $B_3 = -(1/4)\{\delta^5[z^2 + 10(4\beta_1 + 4\beta_2)]$ $+ z^2[(4\beta_1)^2 + (4\beta_2)^2 + 12 \times 4\beta_1 4\beta_2]\}$ $B_4 = (1/12)\delta^4[35 + 45z^2(4\beta_1 + 4\beta_2)]$ $+ (1/48)z^4\delta^4[(4\beta_1)^2 + (4\beta_2)^2 + 12 \times 4\beta_1 4\beta_2]$ $B_5 = -(35/6)\delta^3 z^2 - (5/8)\delta^3 z^4(4\beta_1 + 4\beta_2)$ $B_6 = -(1/24)\delta^2 z^2[(1/2)z^2(4\beta_1 + 4\beta_2) + 35]$ $B_7 = -(7/72)\delta z^6$ $B_8 = (1/4!)^2 z^8$
34	33	(33, 34)			
34	34	(33, 33)			
34	35	(33, 35)			

Notes about table 4

(1) The suffixes i and j correspond to suffix sets (g_1, j_1, k_1) and (g_2, j_2, k_2), respectively. Their relations were presented in table 1.

(2) The difinition of B_ν in table 4 is as follow:

$$B_\nu = B_{r_1,r_2,u} B_{s_1,s_2,\nu} B_{t_1,t_2,w} / C_{ij}. \tag{B.1}$$

The suffix ν was difined in equation (3.3). The first contant expression of every matrix term is the common coefficient of B_ν. This coefficient C_{ij} was defined as

$$C_{ij} = C_{g_1,g_2} C_{j_1,j_2} C_{k_1,k_2}. \tag{B.2}$$

The difinition of C_{g_1,g_2} refers to the formula (A.1) in appendix A.

(3) As shown in figure 4 the shadowy part denotes that these elements were listed in table 4. The other terms of matrix Z' have relations to that listed as follows:

(a)

$$C_{ij} = \begin{cases} C_{ji}; & \text{when } j \text{ is even,} \\ -C_{ji}; & \text{when } j \text{ is odd,} \end{cases} \quad \text{for } i < j. \tag{B.3}$$

(b) For $i < j$, exchange β_1 and β_2 in expressions of B_ν.

(4) The space terms in table 4 are the zero terms of matrix Z'.

(5) The relation between z_{ij} and B_ν is as follow:

$$z_{ij} = C_{ij} \sum_\nu B_\nu F_\nu \left(\frac{\overline{PQ}^2}{4\delta} \right). \tag{B.4}$$

The F function refers to [3].

Appendix C. The rotation matrix

If

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \mathbf{A} \begin{bmatrix} x \\ y \\ z \end{bmatrix},$$

then $\mathbf{X}' = \mathbf{TX}$, where

$$\mathbf{X} = [1\ x\ y\ z\ xy\ xz\ yz\ x^2\ y^2\ z^2\ x^2y\ x^2z\ xy^2\ y^2z\ xz^2\ yz^2\ xyz\ x^3\ y^3\ z^3 \\ x^3y\ x^3z\ xy^3\ y^3z\ xz^3\ yz^3\ x^2y^2\ x^2z^2\ y^2z^2\ x^2yz\ xy^2z\ xyz^2\ x^4\ y^4\ z^4]^{\mathrm{T}},$$

$$\mathbf{T} = \begin{bmatrix} \mathbf{I} & & & & \\ & \mathbf{A} & & & \\ & & \mathbf{B} & & \\ & & & \mathbf{C} & \\ & & & & \mathbf{D} \end{bmatrix},$$

where

$$\mathbf{I} = \mathbf{I}_{1\times 1}, \quad \mathbf{A} = \begin{bmatrix} A & B & C \\ D & E & F \\ G & H & I \end{bmatrix},$$

$$\mathbf{B} = \begin{bmatrix} AE+BD & AF+CD & BF+CE & AD & BE & CF \\ AH+BG & AI+CG & BI+CH & AG & BH & CI \\ DH+EG & DI+FG & EI+FH & DG & GH & FI \\ 2AB & 2AC & 2BC & A^2 & B^2 & C^2 \\ 2DE & 2DF & 2EF & D^2 & E^2 & F^2 \\ 2GH & 2GI & 2HI & G^2 & H^2 & I^2 \end{bmatrix},$$

$$\mathbf{C} = \begin{bmatrix} C_1 & C_2 & C_3 & C_4 & C_5 & C_6 & C_7 & C_8 & C_9 & C_{10} \end{bmatrix}^{\mathrm{T}},$$

$$\begin{aligned}
C_1 = \big[&2ABD + A^2E \;\; 2ACD + A^2F \;\; 2ABE + B^2D \;\; 2BCE + B^2F \\
&2ACF + C^2D \;\; 2BCF + C^2E \;\; 2(ABF + ACF + BCD) \;\; A^2D \;\; B^2E \;\; C^2F\big], \\
C_2 = \big[&2ABG + A^2H \;\; 2ACG + A^2I \;\; 2ABH + B^2G \;\; 2BCH + B^2I \;\; 2ACI + C^2G \\
&2BCI + C^2H \;\; 2(ABI + ACI + BCG) \;\; A^2G \;\; B^2H \;\; C^2I\big], \\
C_3 = \big[&2DEA + D^2B \;\; 2DFA + D^2C \;\; 2DEB + E^2A \;\; 2EFB + E^2C \\
&2DFC + F^2A \;\; 2EFC + F^2B \;\; 2(DEC + DFC + EFA) \;\; D^2A \;\; E^2B \;\; F^2C\big], \\
C_4 = \big[&2DEG + D^2H \;\; 2DFG + D^2I \;\; 2DEH + E^2G \;\; 2EFH + E^2I \\
&2DFI + F^2G \;\; 2EFI + F^2H \;\; 2(DEI + DFI + EFG) \;\; D^2G \;\; E^2H \;\; F^2I\big], \\
C_5 = \big[&2GHA + G^2B \;\; 2GIA + G^2C \;\; 2GHB + H^2A \;\; 2HIB + H^2C \;\; 2GIC + I^2A \\
&2HIC + I^2B \;\; 2(GHC + GIC + HIA) \;\; G^2A \;\; H^2B \;\; I^2C\big], \\
C_6 = \big[&2GHD + G^2E \;\; 2GID + G^2F \;\; 2GHE + H^2D \;\; 2HIE + H^2F \\
&2GIF + I^2D \;\; 2HIF + I^2E \;\; 2(GHF + GIF + HID) \;\; G^2D \;\; H^2E \;\; I^2F\big], \\
C_7 = \big[&(AE + BD)G + ADH \;\; (AF + CD)G + ADI \;\; (AE + BD)H + BEG \\
&(BF + CE)H + BEI \;\; (AF + CD)I + CFG \;\; (BF + CE)I + CFH \\
&(AE + BD)I + (AF + CD)H + (BF + CE)G \;\; ADG \;\; BEH \;\; CFI\big],
\end{aligned}$$

$$C_8 = \left[3A^2B \;\; 3A^2C \;\; 3AB^2 \;\; 3B^2C \;\; 3AC^2 \;\; 3BC^2 \;\; 6ABC \;\; A^3 \;\; B^3 \;\; C^3\right],$$
$$C_9 = \left[3D^2E \;\; 3D^2F \;\; 3DE^2 \;\; 3E^2F \;\; 3DF^2 \;\; 3EF^2 \;\; 6DEF \;\; D^3 \;\; E^3 \;\; F^3\right],$$
$$C_{10} = \left[3G^2H \;\; 3G^2I \;\; 3GH^2 \;\; 3H^2I \;\; 3GI^2 \;\; 3HI^2 \;\; 6GHI \;\; G^3 \;\; H^3 \;\; I^3\right],$$

$$\mathbf{D} = \left[D_1 \; D_2 \; D_3 \; D_4 \; D_5 \; D_6 \; D_7 \; D_8 \; D_9 \; D_{10} \; D_{11} \; D_{12} \; D_{13} \; D_{14} \; D_{15}\right]^{\mathrm{T}},$$

$$\begin{aligned}
D_1 = \big[&3A^2BD + A^3E \;\; 3A^2CD + A^2F \;\; B^3D + 3AB^2E \;\; 3B^2CD + B^3F \\
&C^3D + 3AC^2F \;\; C^3E + 3BC^2F \;\; 3AB^2D + 3A^2BE \;\; 3AC^2D + 3A^2CF \\
&3BC^2E + 3B^2CF \;\; 6ABCD + 3A^2CE + 3A^2BF \;\; 6ABCE + 3AB^2F \\
&+ 3B^2CD \;\; 6ABCF + 3AC^2E + 3BC^2D \;\; A^3D \;\; B^3E \;\; C^3F\big],
\end{aligned}$$

$$\begin{aligned}
D_2 = \big[&3A^2BG + A^3H \;\; 3A^2CG + A^2I \;\; B^3G + 3AB^2H \;\; 3B^2CG + B^3I \\
&C^3G + 3AC^2I \;\; C^3H + 3BC^2I \;\; 3AB^2G + 3A^2BH \;\; 3AC^2G + 3A^2CI \\
&3BC^2H + 3B^2CI \;\; 6ABCG + 3A^2CH + 3A^2BI \;\; 6ABCH + 3AB^2I \\
&+ 3B^2CG \;\; 6ABCI + 3AC^2H + 3BC^2G \;\; A^3G \;\; B^3H \;\; C^3I\big],
\end{aligned}$$

$$\begin{aligned}
D_3 = \big[&3D^2EA + D^3B \;\; 3D^2FA + D^3C \;\; E^3A + 3DE^2B \;\; 3E^2FA + E^3C \\
&F^3A + 3DF^2C \;\; F^3B + 3EF^2C \;\; 3DE^2A + 3D^2EB \;\; 3DF^2A + 3D^2FC \\
&3EF^2B + 3E^2FC \;\; 6DEFA + 3D^2FB + 3D^2EC \;\; 6DEFB + 3DE^2C \\
&+ 3E^2FA \;\; 6DEFC + 3DF^2B + 3EF^2A \;\; D^3A \;\; E^3B \;\; F^3C\big],
\end{aligned}$$

$$\begin{aligned}
D_4 = \big[&3D^2EG + D^3H \;\; 3D^2FG + D^3I \;\; E^3G + 3DE^2H \;\; 3E^2FG + E^3I \\
&F^3G + 3DF^2I \;\; F^3H + 3EF^2I \;\; 3DE^2G + 3D^2EH \;\; 3DF^2G + 3D^2FI \\
&3EF^2H + 3E^2FI \;\; 6DEFG + 3D^2FH + 3D^2EI \;\; 6DEFH + 3DE^2I \\
&+ 3E^2FG \;\; 6DEFI + 3DF^2H + 3EF^2G \;\; D^3G \;\; E^3H \;\; F^3I\big],
\end{aligned}$$

$$\begin{aligned}
D_5 = \big[&3G^2HA + G^3B \;\; 3G^2IA + G^3C \;\; H^3A + 3GH^2B \;\; 3H^2IA + H^3C \\
&I^3A + 3GI^2C \;\; I^3B + 3HI^2C \;\; 3GH^2A + 3G^2HB \;\; 3GI^2A + 3G^2IC \\
&3HI^2B + 3H^2IC \;\; 6GHIA + 3G^2IB + 3G^2HC \;\; 6GHIB + 3GH^2C \\
&+ 3H^2IA \;\; 6GHIC + 3GI^2B + 3HI^2A \;\; G^3A \;\; H^3B \;\; I^3C\big],
\end{aligned}$$

$$\begin{aligned}
D_6 = \big[&3G^2HD + G^3E \;\; 3G^2ID + G^3F \;\; H^3D + 3GH^2E \;\; 3H^2ID + H^3F \\
&I^3D + 3GI^2F \;\; I^3E + 3HI^2F \;\; 3GH^2D + 3G^2HE \;\; 3GI^2D + 3G^2IF \\
&3HI^2E + 3H^2IF \;\; 6GHID + 3G^2IE + 3G^2HF \;\; 6GHIE + 3GH^2F \\
&+ 3H^2ID \;\; 6GHIF + 3GI^2E + 3HI^2D \;\; G^3D \;\; H^3E \;\; I^3F\big],
\end{aligned}$$

$$\begin{aligned}
D_7 = \big[&2ABD^2 + 2A^2DE \;\; 2A^2DF + 2ACD^2 \;\; 2B^2DE + 2ABE^2 \\
&2B^2EF + 2BCE^2 \;\; 2ACF^2 + 2C^2DF \;\; 2C^2EF + 2BCF^2 \\
&4ABDE + B^2D^2 + A^2E^2 \;\; 4ACDF + C^2D^2 + A^2F^2 \\
&4BCEF + C^2E^2 + B^2F^2 \;\; 4ACDE + 4ABDF + 2A^2EF + 2BCD^2
\end{aligned}$$

$$4BCDE + 4ABEF + 2B^2DF + 2ACE^2 \;\; 4ACEF + 4BCDF + 2ABF^2$$
$$+ 2ACE^2 \;\; A^2D^2 \;\; B^2E^2 \;\; C^2F^2\big],$$

$$D_8 = \big[2ABG^2 + 2A^2GH \;\; 2A^2GI + 2ACG^2 \;\; 2B^2GH + 2ABH^2$$
$$2B^2HI + 2BCH^2 \;\; 2ACI^2 + 2C^2GI \;\; 2C^3HI + 2BCI^2$$
$$4ABGH + B^2G^2 + A^2H^2 \;\; 4ACGI + C^2G^2 + A^2I^2$$
$$4BCHI + C^2H^2 + B^2I^2 \;\; 4ACGH + 4ABGI + 2A^2HI + 2BCG^2$$
$$4BCGH + 4ABHI + 2B^2GI + 2ACH^2 \;\; 4ACHI + 4BCGI + 2ABI^2$$
$$+ 2ACH^2 \;\; A^2G^2 \;\; B^2H^2 \;\; C^2I^2\big],$$

$$D_9 = \big[2ABG^2 + 2A^2GH \;\; 2A^2GI + 2ACG^2 \;\; 2B^2GH + 2ABH^2$$
$$2B^2HI + 2BCH^2 \;\; 2ACI^2 + 2C^2GI \;\; 2C^3HI + 2BCI^2$$
$$4ABGH + B^2G^2 + A^2H^2 \;\; 4ACGI + C^2G^2 + A^2I^2$$
$$4BCHI + C^2H^2 + B^2I^2 \;\; 4ACGH + 4ABGI + 2A^2HI + 2BCG^2$$
$$4BCGH + 4ABHI + 2B^2GI + 2ACH^2 \;\; 4ACHI + 4BCGI + 2ABI^2$$
$$+ 2ACH^2 \;\; A^2G^2 \;\; B^2H^2 \;\; C^2I^2\big],$$

$$D_{10} = \big[A^2(DH + EG) + 2ABDG \;\; A^2(DI + FG) + 2ACDG$$
$$B^2(DH + EG) + 2ABEH \;\; B^2(EI + FH) + 2BCEH$$
$$C^2(DI + FG) + 2ACFI \;\; C^2(EI + FH) + 2BCFI$$
$$2AB(DH + EG) + B^2DG + A^2EH \;\; 2AC(DI + FG) + C^2DG + A^2FI$$
$$2BC(EI + FH) + C^2EH + B^2FI \;\; 2AC(DH + EG) + 2AB(DI + FG)$$
$$+ A^2(EI + FH) + 2BCDG \;\; 2BC(DH + EG) + 2AB(EI + FH)$$
$$+ B^2(DI + FG) + 2ACEH \;\; 2AC(EI + FH) + 2BC(DI + FG)$$
$$+ C^2(DH + EG) + 2ABFI \;\; A^2DG \;\; B^2EH \;\; C^2FI\big],$$

$$D_{11} = \big[D^2(AH + BG) + 2DEAG \;\; D^2(AI + CG) + 2GFAG$$
$$E^2(AH + BG) + 2DEBH \;\; E^2(BI + CH) + 2EFBH$$
$$F^2(AI + CG) + 2DFCI \;\; F^2(BI + CH) + 2EFCI$$
$$2DE(AH + BG) + E^2AG + D^2BH \;\; 2DF(AI + CG) + F^2AG + D^2CI$$
$$2EF(BI + CH) + F^2BH + E^2CI \;\; 2DF(AH + BG) + 2DE(AI + CG)$$
$$+ D^2(BI + CH) + 2EFAG \;\; 2EF(AH + BG) + 2DE(BI + CH)$$
$$+ E^2(AI + CG) + 2DFBH \;\; 2DF(BI + CH) + 2EF(AI + CG)$$
$$+ F^2(AH + BG) + 2DECI \;\; D^2AG \;\; E^2BH \;\; F^2CI\big],$$

$$D_{12} = \big[G^2(AE + BD) + 2GHAD \;\; G^2(AF + CD) + 2DIAD$$
$$H^2(AE + BD) + 2GHBE \;\; H^2(BF + CE) + 2HIBE$$
$$I^2(AF + CD) + 2GICF \;\; I^2(BF + CE) + 2HICF$$
$$2GH(AE + BD) + H^2AD + G^2BE \;\; 2GI(AF + CD) + I^2AD + G^2CF$$

$$
\begin{aligned}
&2HI(BF+CE)+I^2BE+H^2CF\ \ 2GI(AE+BD)+2GH(AF+CD)\\
&+G^2(BF+CE)+2HIAD\ \ 2HI(AE+BD)+2GH(BF+CE)\\
&+H^2(AF+CD)+2GIBE\ \ 2GI(BF+CE)+2HI(AF+CD)\\
&+I^2(AE+BD)+2GHCF\ \ G^2AD\ \ H^2BE\ \ I^2CF\big],
\end{aligned}
$$

$$
\begin{aligned}
D_{13}=\big[&4A^3B\ \ 4A^3C\ \ 4AB^3\ \ 4B^3C\ \ 4AC^3\ \ 4BC^3\ \ 6A^2B^2\ \ 6A^2C^2\ \ 6B^2C^2\\
&12A^2BC\ \ 12AB^2C\ \ 12ABC^2\ \ A^4\ \ B^4\ \ C^4\big],\\
D_{14}=\big[&4D^3E\ \ 4D^3F\ \ 4DE^3\ \ 4E^3F\ \ 4DF^3\ \ 4EF^3\ \ 6D^2E^2\ \ 6D^2F^2\ \ 6E^2F^2\\
&12D^2EF\ \ 12DE^2F\ \ 12DEF^2\ \ D^4\ \ E^4\ \ F^4\big],\\
D_{15}=\big[&4G^3H\ \ 4G^3I\ \ 4GH^3\ \ 4H^3I\ \ 4GI^3\ \ 4HI^3\ \ 6G^2H^2\ \ 6G^2I^2\ \ 6H^2I^2\ \ 12G^2HI\\
&12GH^2I\ \ 12GHI^2\ \ G^4\ \ H^4\ \ I^4\big].
\end{aligned}
$$

References

[1] D.M. Bishop, *Group Theory and Chemistry* (Clarendon Press, Oxford, 1973) p. 184.
[2] M. Dupuis, J. Rys and H.F. King, J. Comput. Phys. 65 (1976) 111.
[3] P.M.W. Gill, Adv. Quantum Chem. 25 (1994) 141.
[4] P.M.W. Gill, M. Head-Gorden and J.A. Pople, J. Phys. Chem. 94 (1990) 5564.
[5] M. Head-Gorden and J.A. Pople, J. Chem. Phys. 89 (1988) 5777.
[6] H.F. King and M. Dupuis, J. Comput. Phys. 21 (1976) 144.
[7] L.E. McMurchie and E.R. Davidson, J. Comput. Phys. 26 (1978) 218.
[8] D.H. Mooley, J.G. Fripial, B. Champague and J.M. Andre, Int. J. Quantum Chem., Quantum Chem. Symp. 27 (1993) 793.
[9] S. Obara and H. Saika, J. Chem. Phys. 84 (1986) 3963.
[10] J.A. Pople and W.J. Hehre, J. Comput. Phys. 27 (1978) 161.
[11] J. Rys, M. Dupuis and H.F. King, J. Comput. Chem. 4 (1983) 154.