J Math Chem (2008) 44:28–45
DOI 10.1007/s10910-007-9290-2

ORIGINAL PAPER

Evaluation of recurrence relationships and numerical solutions for finite rotation matrix elements by using auxiliary functions

E. Öztekin · S. Özcan

Received: 28 March 2007 / Accepted: 13 July 2007 / Published online: 2 September 2007

Abstract In this article, we derived several new recurrence relations of the rotation matrix elements by using Gauss' recurrence formulas for hypergeometric functions and auxiliary functions $A^{j}_{m',m}(\beta)$, and $B^{k}_{i,l}(\beta)$. The aim of this contribution is to obtain general algorithm to compute the rotation matrix elements, paying attention to the use recurrence relationships of the auxiliary functions that allow the treatment of the functions with high angular momentum quantum numbers.

Keywords Rotation matrix elements · Auxiliary functions for $d^{j}_{m',m}(\beta)$ · Hypergeometric functions · Gauss' recurrence formulas

1 Introduction

The matrix representations of finite rotations play an important role in the theory of angular momentum. In quantum chemistry and physics, they occur for instances as factor of applications of these molecular spectroscopy. Their many properties and derivations have been investigated by Edmonds [1], Fano and Racah [2], Rose [3], and Altmann and Bradley [4].

The Wigner D functions and their properties can be easily found in the literature. In order to determine the matrix representation of the rotation operator, three parameters are needed to specify a rotation. The most useful description is, however, in terms of Euler angles, which we shall called α, β, and γ. The dependence on α and γ of the matrix representation of the rotation operator R can be determined very simply. We shall follow the notation of Ref. [3]. The elements of the finite rotation matrix can be

E. Öztekin (✉) · S. Özcan
Department of Physics, Faculty of Science and Arts, University of Ondokuz Mayis, Kurupelit, Samsun 55139, Turkey
e-mail: eminoz@omu.edu.tr

make dependent of them through

$$D^{j}_{m',m}(\alpha\beta\gamma) = e^{-im'\alpha}\left\langle jm'\right| e^{-i\beta J_y}\left|jm\right\rangle e^{-im\gamma} = e^{-im'\alpha} d^{j}_{m',m}(\beta) e^{-im\gamma} \tag{1}$$

The $d^{j}_{m',m}(\beta)$ matrix can be put in closed form as [3],

$$d^{j}_{m',m}(\beta) = \left\{\frac{F_m\left(j+m\right)F_{m'}\left(j+m'\right)}{F_m\left(j\right)F_{m'}\left(j\right)}\right\}^{1/2}\left(\cos\frac{\beta}{2}\right)^{2j} \times \sum_i (-1)^{i+m'-m}\frac{F_m\left(m'+i\right)F_{i-m}\left(j\right)F_{m'+i}\left(j\right)}{F_m\left(i\right)}\left(\tan\frac{\beta}{2}\right)^{m'-m+2i} \tag{2}$$

Where $F_m\left(n\right)$ are binomial coefficients and i runs through all integer values for which the factorials involved exists. $d^{j}_{m',m}(\beta)$ coefficients have the following symmetry properties [3];

$$d^{j}_{m',m}(\beta) = d^{j}_{m,m'}(-\beta) = (-1)^{m-m'} d^{j}_{m,m'}(\beta) = (-1)^{m-m'}\left(d^{j}_{m',m}(\beta)\right)^{*} = d^{j}_{-m,-m'}(\beta) = (-1)^{m-m'} d^{j}_{-m',-m}(\beta) \tag{3}$$

Because the Wigner rotation matrix elements involve the sum of the binomial coefficients the calculation involving them is tedious. It is more interesting to obtain these matrix elements by means of recurrence relationships as happened with many polynomials. To accomplish this task, we will use the fact that $d^{j}_{m',m}(\beta)$ matrix element rewritten as multiplied of two new functions as $A^{j}_{m',m}(\beta)$ and $B^{k}_{i,l}(\beta)$ which we called auxiliary functions for $d^{j}_{m',m}(\beta)$. In Sect. 3, the quantitative relations for $A^{j}_{m',m}(\beta)$ and $B^{k}_{i,l}(\beta)$ are formalized. In the present paper, firstly, we establish to $A^{j}_{m',m}(\beta)$ and recurrence relationships by represented with $N^{j}_{m'}P^{m'}_{m'}(\cos\beta)\,A^{j}_{0,m}(\beta)$. The required background mathematics is assembled in Sect. 3.1. In this case, $A^{j}_{0,m}(\beta)$ functions for a given m and j values are common for all m' values. This gives us the advantage for lower CPU times. Thus, the computation is faster. In Sect. 3.2., using the Gauss' recurrence formula of hypergeometric functions, we obtained many recurrence relations for $B^{k}_{i,l}(\beta)$. Using recurrence relationships for auxiliary functions, we are able to easily calculate useful recurrence relations and special values for $d^{j}_{m',m}(\beta)$. Detailed derivations will be found in the Sect. 4.

The final Section provides information about the computational implementation and documentation of the advantages of the new approach as regards speed and accuracy.

2 Definitions and basic properties

The associated Legendre polynomials $P_l^m(x)$ are defined in terms of the Legendre polynomials $P_l(x)$ by

$$P_l^m(x) = \left(1 - x^2\right)^{m/2} \frac{d^m}{dx^m} P_l(x) = \frac{1}{2^l l!} \left(1 - x^2\right)^{m/2} \frac{d^{l+m}}{dx^{l+m}} \left(x^2 - 1\right)^l \tag{4}$$

Where m is a positive integer $m = 0, 1, 2, \ldots l$ [5]. For $m = l$, associated Legendre polynomials are given

$$P_l^l(x) = (2l - 1)!! \left(1 - x^2\right)^{l/2} = (2l - 1) \sqrt{1 - x^2} P_{l-1}^{l-1}(x) \tag{5}$$

A generalized hypergeometric series is given by

$${}_pF_q\left(a_1, a_2, \ldots a_p; b_1, b_2, \ldots b_q; z\right) = \sum_{k=0}^{\infty} \frac{(a_1)_k (a_2)_k \ldots \left(a_p\right)_k z^k}{(b_1)_k (b_2)_k \ldots \left(b_q\right)_k k!} \tag{6}$$

Where $(a)_k$ stands for the Pochhammer symbol which may be defined in terms of Gamma function $\Gamma(z)$ according to [6];

$$(a)_k = \frac{\Gamma(a + k)}{\Gamma(a)} = a(a + 1) \ldots (a + k - 1)$$

Transformation formulas for hypergeometric functions

$$F(a, b; c; z) = (1 - z)^{-a} F\left(a, c - b; c; \frac{z}{z - 1}\right) = (1 - z)^{-b} F\left(b, c - a; c; \frac{z}{z - 1}\right) = (1 - z)^{c-a-b} F(c - a, c - b; c; z) \tag{7}$$

Particular values

$$F(a, b; c; 1) = \frac{\Gamma(c)\Gamma(c - a - b)}{\Gamma(c - a)\Gamma(c - b)} \quad \text{for} \quad \mathrm{Re}c > \mathrm{Re}(a + b) = F(-a, -b; c - a - b; 1) = \frac{1}{F(-a, b; c - a; 1)} = \frac{1}{F(a, -b; c - b; 1)} \tag{8}$$

The Jacobi polynomials $\wp_n^{(\alpha,\beta)}(x)$ may be expressed in terms of hypergeometric functions as follows [6];

$$\wp_n^{(\alpha,\beta)}(x) = \frac{(-1)^n\,\Gamma(n+1+\beta)}{n!\Gamma(1+\beta)} F\left(n+\alpha+\beta+1, -n; 1+\beta; \frac{1+x}{2}\right) \tag{9.a}$$

$$= \frac{\Gamma(n+1+\alpha)}{n!\Gamma(1+\alpha)} F\left(n+\alpha+\beta+1, -n; 1+\alpha; \frac{1-x}{2}\right) \tag{9.b}$$

$$= \frac{\Gamma(n+1+\alpha)}{n!\Gamma(1+\alpha)} \left(\frac{1+x}{2}\right)^n F\left(-n, -n-\beta; \alpha+1; \frac{x-1}{x+1}\right) \tag{9.c}$$

$$= \frac{\Gamma(n+1+\beta)}{n!\Gamma(1+\beta)} \left(\frac{x-1}{2}\right)^n F\left(-n, -n-\alpha; \beta+1; \frac{x+1}{x-1}\right) \tag{9.d}$$

Rotation coefficients are given in terms of Jacobi polynomials [1];

$$d^j_{m',m}(\beta) = \left\{\frac{(j+m')!\,(j-m')!}{(j+m)!\,(j-m)!}\right\}^{1/2} \left(\cos\frac{\beta}{2}\right)^{m'+m} \times \left(\sin\frac{\beta}{2}\right)^{m'-m} \wp_{j-m'}^{(m'-m,m'+m)}(\cos\beta) \tag{10}$$

3 Auxiliary functions for rotation matrix elements

All subsequent derivations are deduced from the following definitions

$$d^j_{m',m}(\beta) = A^j_{m',m}(\beta) B^k_{i,l}(\beta) \tag{11}$$

By using Eqs. 9.d, 10 and 11, we denote following auxiliary functions for $d^j_{m'm}(\beta)$ matrices elements

$$A^j_{m',m}(\beta) = \left[\frac{(j+m)!\,(j+m')!}{(j-m)!\,(j-m')!}\right]^{1/2} \left(\cos\frac{\beta}{2}\right)^{m+m'} \left(\sin\frac{\beta}{2}\right)^{m'-m} \tag{12}$$

$$B^k_{i,l}(\beta) = \frac{1}{\Gamma(k)} \left(\frac{2}{\cos\beta-1}\right)^i {}_2F_1\left(i, l; k; \frac{\cos\beta+1}{\cos\beta-1}\right) \tag{13}$$

where we denote $i = m'-j$, $l = m-j$, and $k = m+m'+1$.

To determine the recurrence relationships of the $d^j_{m',m}(\beta)$, we proceed in two main steps; (1) the determination of $A^j_{m',m}(\beta)$, and (2) the development of $B^k_{i,l}(\beta)$ by using Gauss' recurrence formula for the hypergeometric functions. These relationships are developed in following Section.

3.1 Formulas for $A^{j}_{m',m}(\beta)$

More information about the behaviour of the $A^{j}_{m',m}(\beta)$ can be obtained by using properties of the associated Legendre functions with $m = l$ [5]. Some mathematical manipulations in Eq. 12, $A^{j}_{m',m}(\beta)$ can be rewritten as following form

$$A^{j}_{m',m}(\beta) = \frac{(m')!}{(2m')!}\left[\frac{(j+m')!}{(j-m')!}\right]^{1/2} P^{m'}_{m'}(\cos\beta)\, A^{j}_{0,m}(\beta) \tag{14}$$

With these relationships, one can obtain the multiplied with the Legendre polynomials and $A^{j}_{0,m}(\beta)$, so that no one expression is computed more than once, because only Legendre polynomials with $m' \geq 0$ are needed, and $A^{j}_{0,m}(\beta)$ functions for a given m and j are common for all m' values. The normalization factors can be computed at very beginning of a calculation. Where

$$A^{j}_{m,0}(\beta) = \frac{1}{2^{m}\,(2m-1)!!}\sqrt{\frac{(j+m)!}{(j-m)!}}\, P^{m}_{m}(\cos\beta) \tag{15}$$

For $m = m'$, Eq. 14 becomes

$$A^{j}_{m,m}(\beta) = \frac{1}{2^{m}}\frac{(j+m)!}{(j-m)!}\left(A^{1}_{1,1}(\beta)\right)^{m} \tag{16}$$

From Eqs. 14 and 15 numerous additional recurrence relationships may be developed, including;

$$\begin{aligned} A^{j}_{m',m}(\beta) &= \frac{1}{2}\left[\left(j+m'\right)\left(j-m'+1\right)\right]^{1/2}\sin\beta\, A^{j}_{m'-1,m}(\beta) \\ &= \left[(j-m+1)\,(j+m)\right]^{1/2}\cot\frac{\beta}{2}\, A^{j}_{m',m-1}(\beta) \qquad (17) \\ &= \sqrt{\frac{(j+m)\,(j+m')}{(j-m)\,(j-m')}}\, A^{j-1}_{m',m}(\beta) \qquad (18) \end{aligned}$$

$$\begin{aligned} A^{j+1}_{m'+1,m+1}(\beta) &= \left[(j+m+2)\,(j+m+1)\left(j+m'+2\right)\left(j+m'+1\right)\right]^{1/2} \\ &\quad\times\cos^{2}\frac{\beta}{2}\, A^{j}_{m',m}(\beta) \qquad (19) \\ A^{j}_{m'+1,m+1}(\beta) &= \left[(j+m+1)\left(j+m'+1\right)\left(j-m'\right)(j-m)\right]^{1/2} \\ &\quad\times\cos^{2}\frac{\beta}{2}\, A^{j}_{m',m}(\beta) \qquad (20) \end{aligned}$$

The $A^{j}_{m',m}(\beta)$ functions have the following symmetry properties and special values;

$$A^{j}_{m,m'}(\beta) = \left(\sin^2 \frac{\beta}{2}\right)^{m-m'} A^{j}_{m',m}(\beta) \tag{21}$$

$$A^{j}_{m',m}(\beta) A^{j}_{-m',-m}(\beta) = 1 \tag{22}$$

$$A^{j}_{m',m}(-\beta) = (-1)^{m'-m} A^{j}_{m',m}(\beta) \tag{23}$$

$$A^{j}_{m',m}(\pi + \beta) = (-1)^{m'+m} \frac{(j+m)!}{(j-m)!} A^{j}_{m',-m}(\beta) \tag{24}$$

$$A^{j}_{m',m}(\pi - \beta) = \frac{(j+m)!}{(j-m)!} A^{j}_{m',-m}(\beta) \tag{25}$$

$$A^{j}_{m',m}(0) = \frac{(j+m)!}{(j-m)!} \delta_{m',m} \tag{26}$$

$$A^{j}_{m',m}(\pi) = \delta_{-m,m'} \tag{27}$$

The behaviours of $A^{j}_{m',m}(\beta)$, which contain β and quantum numbers dependences, are illustrated in Fig. 1. As can be seen from Fig. 1, $A^{j}_{m',m}(\beta)$ have following values in initial and final points of β.

1. Case, $\beta = 0$:
   a. When $m = m'$, all $A^{j}_{m',m}(0) \neq 0$,
   b. When $m < m'$, all $A^{j}_{m',m}(0) = 0$,
   c. When $m > m'$, all $A^{j}_{m',m}(0) \to \infty$
2. Case, $\beta = \pi$:
   a. When $m = -m'$, all $A^{j}_{m',m}(\pi) \neq 0$,
   b. When $|m'| > |-m|$ or $|m| > |-m'|$, $A^{j}_{m',m}(\pi) \to \infty$,
   c. When $m = m'$, all $A^{j}_{m',m}(\pi) = 0$,
   d. When $m < m'$, $A^{j}_{m',m}(\pi) = 0$,

3.2 Recurrence relations and special values for $B^{k}_{i,l}(\beta)$

The recurrence relations for $B^{k}_{i,l}(\beta)$ can be obtained properties of hypergeometric functions and by using Gauss' recurrence formulas. We use here the definitions given by Gradshteyn and Ryzhik [6]. After some mathematical manipulations in Eq. 13, we obtained following recurrence relationships for $B^{k}_{i,l}(\beta)$;

$$\left[(k-1)\sin^2 \frac{\beta}{2} + (2k-i-l-1)\cos^2 \frac{\beta}{2}\right] B^{k}_{i,l}(\beta) = (k-i)(k-l)\cos^2 \frac{\beta}{2} B^{k+1}_{i,l}(\beta) + B^{k-1}_{i,l}(\beta) \tag{28}$$

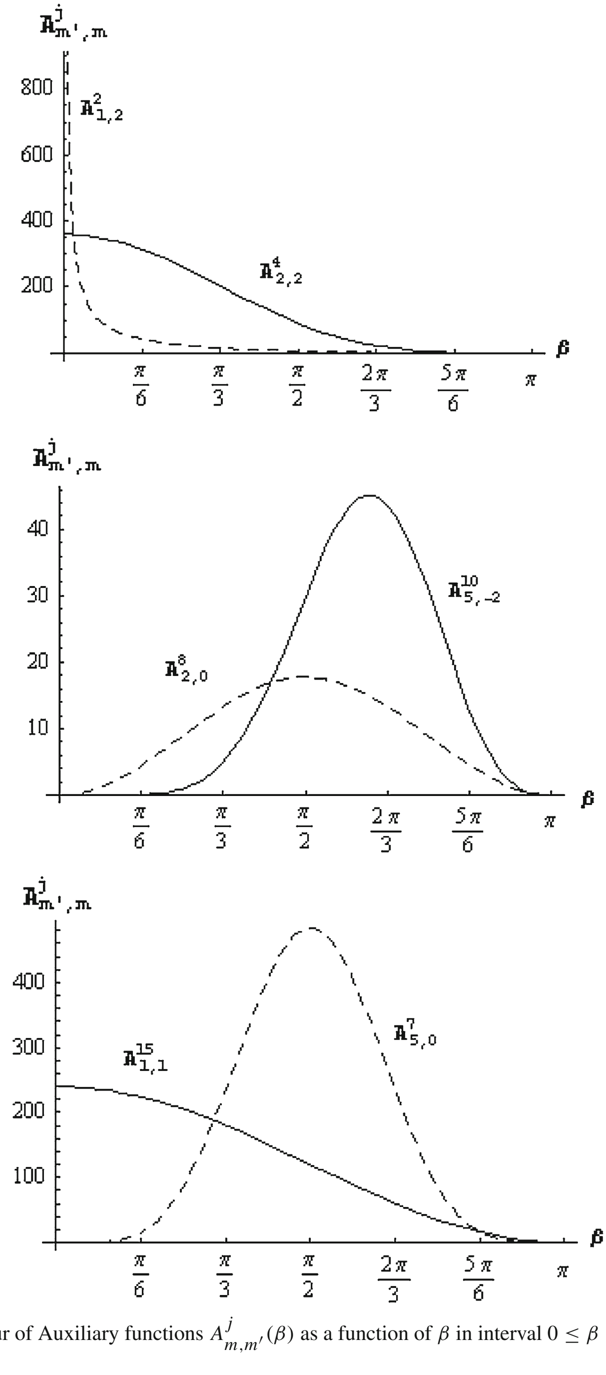

Fig. 1 Behaviour of Auxiliary functions $A^{j}_{m,m'}(\beta)$ as a function of β in interval $0 \le \beta \le \pi$

$$\left[(2i-k)\sin^2\frac{\beta}{2}+(i-l)\cos^2\frac{\beta}{2}\right]B^k_{i,l}(\beta)$$
$$=(k-i)\,B^k_{i-1,l}(\beta)-i\sin^2\frac{\beta}{2}B^k_{i+1,l}(\beta) \tag{29}$$
$$\left[(2l-k)\sin^2\frac{\beta}{2}+(l-i)\cos^2\frac{\beta}{2}\right]B^k_{i,l}(\beta)$$
$$=(l-k)\sin^2\frac{\beta}{2}B^k_{i,l-1}(\beta)+l\,B^k_{i,l+1}(\beta) \tag{30}$$
$$\sin^2\frac{\beta}{2}B^k_{i,l-1}(\beta)=(i-l)\cos^2\frac{\beta}{2}B^{k+1}_{i,l}(\beta)-B^k_{i-1,l}(\beta) \tag{31}$$
$$(i-l)\,B^k_{i,l}(\beta)=i\,(l-k)\sin^2\frac{\beta}{2}B^{k+1}_{i+1,l}(\beta)+l\,(i-k)\,B^{k+1}_{i,l+1}(\beta) \tag{32}$$
$$B^k_{i,l}(\beta)=kB^{k+1}_{i,l}(\beta)+il\cos^2\frac{\beta}{2}B^{k+2}_{i+1,l+1}(\beta) \tag{33}$$
$$B^k_{i,l}(\beta)=(k-i)\,B^{k+1}_{i,l+1}(\beta)-i\,B^{k+1}_{i+1,l+1}(\beta) \tag{34}$$
$$B^k_{i,l}(\beta)=(l-k)\sin^2\frac{\beta}{2}B^{k+1}_{i+1,l}(\beta)-l\,B^{k+1}_{i+1,l+1}(\beta) \tag{35}$$
$$\left[(k-i)\sin^2\frac{\beta}{2}+l\cos^2\frac{\beta}{2}\right]B^k_{i,l}(\beta)$$
$$=(i-k)\,B^k_{i-1,l}(\beta)-il\cos^2\frac{\beta}{2}B^{k+1}_{i+1,l+1}(\beta) \tag{36}$$
$$\left[(k-l)\sin^2\frac{\beta}{2}+i\cos^2\frac{\beta}{2}\right]B^k_{i,l}(\beta)$$
$$=(k-l)\sin^2\frac{\beta}{2}B^k_{i,l-1}(\beta)-il\cos^2\frac{\beta}{2}B^{k+1}_{i+1,l+1}(\beta) \tag{37}$$
$$B^k_{i,l}(\beta)=B^k_{i,l+1}(\beta)-i\cos^2\frac{\beta}{2}B^{k+1}_{i+1,l+1}(\beta) \tag{38}$$
$$B^k_{i,l}(\beta)=-\sin^2\frac{\beta}{2}B^k_{i+1,l}(\beta)-l\cos^2\frac{\beta}{2}B^{k+1}_{i+1,l+1}(\beta) \tag{39}$$
$$\left[i\sin^2\frac{\beta}{2}+(k-l)\cos^2\frac{\beta}{2}\right]B^k_{i,l}(\beta)$$
$$=(k-i)\,(k-l)\cos^2\frac{\beta}{2}B^{k+1}_{i,l}(\beta)-i\sin^2\frac{\beta}{2}B^k_{i+1,l}(\beta) \tag{40}$$
$$\left[l\sin^2\frac{\beta}{2}+(k-i)\cos^2\frac{\beta}{2}\right]B^k_{i,l}(\beta)$$
$$=l\,B^k_{i,l+1}(\beta)+(k-i)\,(k-l)\cos^2\frac{\beta}{2}B^{k+1}_{i,l}(\beta) \tag{41}$$
$$B^k_{i,l}(\beta)=kB^{k+1}_{i,l+1}(\beta)-i\,(k-l)\cos^2\frac{\beta}{2}B^{k+2}_{i+1,l+1}(\beta) \tag{42}$$
$$B^k_{i,l}(\beta)=-k\sin^2\frac{\beta}{2}B^{k+1}_{i+1,l}(\beta)+l\,(i-k)\cos^2\frac{\beta}{2}B^{k+2}_{i+1,l+1}(\beta) \tag{43}$$
$$B^k_{i,l}(\beta)=(k-l)\,B^{k+1}_{i,l}(\beta)+l\,B^{k+1}_{i,l+1}(\beta) \tag{44}$$

$$B_{i,l}^{k}(\beta) = (k-i)\, B_{i,l}^{k+1}(\beta) - i\,\sin^2\frac{\beta}{2}\, B_{i+1,l}^{k+1}(\beta) \tag{45}$$

By using Eq. 13 and the properties of hypergeometric functions, $B_{i,l}^{k}(\beta)$ functions may be represented also as following special values;

$$B_{i,l}^{k}(\beta) = (-1)^{k-i}\left(\sin^2\frac{\beta}{2}\right)^{i-l} B_{k-i,k-l}^{k}(\beta) \tag{46}$$

$$B_{i,l}^{k}(-\beta) = B_{i,l}^{k}(\beta) \tag{47}$$

$$B_{i,l}^{k}(\pi+\beta) = (-1)^{j-m}\frac{(j-m')!}{(j+m')!}\left(\cot^2\frac{\beta}{2}\right)^{m}\left(\frac{2}{\sin\beta}\right)^{2m'} B_{l-k+1,l}^{l-i+1}(\beta) \tag{48}$$

$$B_{i,l}^{k}(\pi-\beta) = (-1)^{j-m'}\frac{(j-m')!}{(j+m')!}\left(\cos^2\frac{\beta}{2}\right)^{m-m'} B_{l,l-k+1}^{l-i+1}(\beta) \tag{49}$$

$$\begin{aligned} B_{i,l}^{k}\left(\frac{\pi}{2}\right) &= (-2)^{i}\frac{\Gamma(k-i-l)}{\Gamma(k-i)\,\Gamma(k-l)} \\ &= 2^{2i}\frac{\Gamma(k-i-l)}{\Gamma(i)} B_{-i,-l}^{k-i-l}\left(\frac{\pi}{2}\right) \\ &= \frac{1}{\Gamma(k)\,\Gamma(k-i)\, B_{-i,l}^{k-l}\left(\frac{\pi}{2}\right)} = \frac{1}{2^{-i}\Gamma(k)\,\Gamma(k-l)\, B_{i,-l}^{k-l}\left(\frac{\pi}{2}\right)} \end{aligned} \tag{50}$$

$$\lim_{k\to -n} B_{i,l}^{k}(\beta) = (i)_{n+1}\,(l)_{n+1}\left(\cos^2\frac{\beta}{2}\right)^{n+1} B_{i+n+1,l+n+1}^{n+2}(\beta) \tag{51}$$

Where $(a)_n$ is the Pochhammer symbol and $n = 0, 1, 2, \ldots$

In Fig. 2, we present behaviour of some $B_{i,l}^{k}(\beta)$ in different quantum numbers and interval $\beta = 0 - \pi$.

These will be elements of the lower of the $B_{0,0}^{0}(\beta)$, $B_{1,1}^{1}(\beta)$, $B_{1,0}^{1}(\beta)$, and $B_{0,1}^{1}(\beta)$ matrices elements. The first one is the simplest;

$$\begin{aligned} B_{0,0}^{0}(\beta) &= 0 \\ B_{1,0}^{1}(\beta) &= \frac{2}{Cos\beta - 1} \\ B_{1,1}^{1}(\beta) &= -1 \\ B_{0,1}^{1}(\beta) &= 1 \end{aligned} \tag{52}$$

Collecting Eqs. 28–30 and 52, the following algorithm to obtain $B_{i,l}^{k}(\beta)$ elements can be derived [7,8];

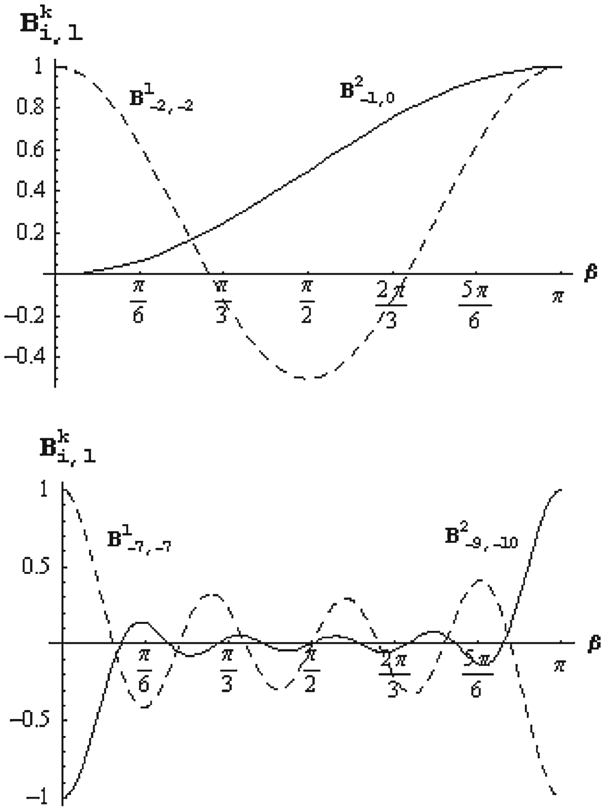

Fig. 2 Behaviour of Auxiliary functions $B_{i,l}^{k}(\beta)$ as a function of β

Read N, R, S, and β
obtain $B_{0,0}^{0}(\beta)$, $B_{0,1}^{1}(\beta)$, $B_{1,0}^{1}(\beta)$, and$B_{1,1}^{1}(\beta)$ from Eqs. 52
    for k = 0, N, 1
        let L = k
        for i = k, R, 1
            obtain $B_{i+1,l}^{k}(\beta)$ by using Eq. 29
        end for (i)
        let i = k
        for L = k, S,1
            obtain $B_{i,l+1}^{k}(\beta)$ by using Eq. 30
        end for (L)
        let L = k
        obtain $B_{i,l}^{k+1}(\beta)$ by using Eq. 28
    end for(k)

In this way all elements of the $B_{i,l}^{k}(\beta)$ of all order can be computed. With these recurrence relationships given by Eqs. 17–20 and 28–45, one can obtain the recurrence formulas for $A^{j}_{m',m}(\beta)$ and Gauss recurrence formulas for $B^{k}_{i,l}(\beta)$, so that all expressions for $d^{j}_{m',m}(\beta)$ is computed by using Eq. 11.

4 Recurrence relationships of the rotation coefficients by using auxiliary functions

To obtain the recurrence relationships for rotation matrix elements one can use closed formulas for auxiliary functions $A^{j}_{m',m}(\beta)$ and $B^{k}_{i,l}(\beta)$, and then evaluate directly $\sin^{m}\theta$ and $\cos^{m}\theta$. Same time, this can lead to numerical stabilities, in addition to being lowest CPU when as is usually case, all the auxiliary functions up to a given j are needed. In this case, it is more efficient to use stable recurrence relationships, such as

$$\left(m'-m\right)\cot\frac{\beta}{2}d^{j}_{m',m}(\beta)=\left\{j\left(j+1\right)-m'\left(m'+1\right)\right\}^{1/2}d^{j}_{m'+1,m}(\beta)+\left\{j\left(j+1\right)-m\left(m+1\right)\right\}^{1/2}d^{j}_{m',m+1}(\beta) \tag{53}$$

$$\left(m+m'\right)\tan\frac{\beta}{2}d^{j}_{m',m}(\beta)=\left\{j\left(j+1\right)-m\left(m-1\right)\right\}^{1/2}d^{j}_{m',m-1}(\beta)-\left\{j\left(j+1\right)-m'\left(m'+1\right)\right\}^{1/2}d^{j}_{m'+1,m}(\beta) \tag{54}$$

$$\left(m+m'\right)\tan\frac{\beta}{2}d^{j}_{m',m}(\beta)=\left\{j\left(j+1\right)-m\left(m+1\right)\right\}^{1/2}d^{j}_{m',m+1}(\beta)-\left\{j\left(j+1\right)-m'\left(m'-1\right)\right\}^{1/2}d^{j}_{m'-1,m}(\beta) \tag{55}$$

$$\left(m'-m\right)\cot\frac{\beta}{2}d^{j}_{m',m}(\beta)=\left\{j\left(j+1\right)-m'\left(m'-1\right)\right\}^{1/2}d^{j}_{m'-1,m}(\beta)+\left\{j\left(j+1\right)-m\left(m-1\right)\right\}^{1/2}d^{j}_{m',m-1}(\beta) \tag{56}$$

$$\left\{(j-m)(j+m)\left(j+m'\right)\right\}^{1/2}d^{j}_{m',m}(\beta)=j\left(j+m'-1\right)^{1/2}\sin\beta d^{j-1}_{m'-1,m}(\beta)+(m+j\cos\beta)\left(j-m'\right)^{1/2}d^{j-1}_{m',m}(\beta) \tag{57}$$

$$\left\{(j-m)\left(j-m'\right)\left(j+m'\right)\right\}^{1/2}d^{j}_{m',m}(\beta)=\left(j\cos\beta-m'\right)(j+m)^{1/2}d^{j-1}_{m',m}(\beta)-j\left(j-m-1\right)^{1/2}\sin\beta d^{j-1}_{m',m+1}(\beta) \tag{58}$$

$$\left\{(j+m)\left(j+m'\right)\left(j-m'\right)\right\}^{1/2}d^{j}_{m',m}(\beta)=j\left(j+m-1\right)^{1/2}\sin\beta d^{j-1}_{m',m-1}(\beta)-\left(m'+j\cos\beta\right)(j-m)^{1/2}d^{j-1}_{m',m}(\beta) \tag{59}$$

$$\left\{(j-m)\left(j-m'\right)(j+m)\right\}^{1/2}d^{j}_{m',m}(\beta)=(j\cos\beta-m)\left(j+m'\right)^{1/2}d^{j-1}_{m',m}(\beta)-j\left(j-m'-1\right)^{1/2}\sin\beta d^{j-1}_{m'+1,m}(\beta) \tag{60}$$

$$\left(j+m'\right)^{1/2}\left(m-j\cos\beta\right)d^{j}_{m',m}(\beta)$$
$$=-j\left(j-m'+1\right)^{1/2}\sin\beta d^{j}_{m'-1,m}(\beta)-\left\{(j-m)\left(j-m'\right)(j+m)\right\}^{1/2}d^{j-1}_{m',m}(\beta) \tag{61}$$

$$(j-m)^{1/2}\left(m'+j\cos\beta\right)d^{j}_{m',m}(\beta)$$
$$=j\left(j+m+1\right)^{1/2}\sin\beta d^{j}_{m',m+1}(\beta)+\left\{(j+m)\left(j+m'\right)\left(j-m'\right)\right\}^{1/2}d^{j-1}_{m',m}(\beta) \tag{62}$$

$$(j+m)^{1/2}\left(m'-j\cos\beta\right)d^{j}_{m',m}(\beta)$$
$$=j\left(j-m+1\right)^{1/2}\sin\beta d^{j}_{m',m-1}(\beta)-\left\{(j-m)\left(j+m'\right)\left(j-m'\right)\right\}^{1/2}d^{j-1}_{m',m}(\beta) \tag{63}$$

$$\left(j-m'\right)^{1/2}\left(m+j\cos\beta\right)d^{j}_{m',m}(\beta)$$
$$=-j\left(j+m'+1\right)^{1/2}\sin\beta d^{j}_{m'+1,m}(\beta)+\left\{(j+m)\left(j+m'\right)(j-m)\right\}^{1/2}d^{j-1}_{m',m}(\beta) \tag{64}$$

To continue, we need the recurrence relationships to use in the generation $d^{j}_{m',m}(\beta)\rightarrow d^{j}_{m',m+1}(\beta)+d^{j}_{m',m-1}(\beta)$ matrix elements. Eqs. 53, 54 or 55, 56, one can be written in a more useful form as;

$$\frac{2\left(m'-m\cos\beta\right)}{\sin\beta}d^{j}_{m',m}(\beta)=\left\{j\left(j+1\right)-m\left(m+1\right)\right\}^{1/2}d^{j}_{m',m+1}(\beta)$$
$$+\left\{j\left(j+1\right)-m\left(m-1\right)\right\}^{1/2}d^{j}_{m',m-1}(\beta) \tag{65}$$

To evaluate these elements by means of recurrence release, Eqs. 53, 55 or 54, 56 can be used obtain;

$$\frac{2\left(m'\cos\beta-m\right)}{\sin\beta}d^{j}_{m',m}(\beta)=\left\{j\left(j+1\right)-m'\left(m'+1\right)\right\}^{1/2}d^{j}_{m'+1,m}(\beta)$$
$$+\left\{j\left(j+1\right)-m'\left(m'-1\right)\right\}^{1/2}d^{j}_{m'-1,m}(\beta) \tag{66}$$

In the same way, Eq. 57 and Eq. 61 can be transformed into;

$$(2j+1)\left\{j\left(j+1\right)\cos\beta-m'm\right\}d^{j}_{m',m}(\beta)=$$
$$(j+1)\left\{\left(j^{2}-m^{2}\right)\left(j^{2}-m'^{2}\right)\right\}^{1/2}d^{j-1}_{m',m}(\beta)$$
$$+j\left\{\left((j+1)^{2}-m^{2}\right)\left((j+1)^{2}-m'^{2}\right)\right\}^{1/2}d^{j+1}_{m',m}(\beta) \tag{67}$$

Obtain results given by Eqs. 65–67 are same as Refs. [9–12].

By using Eqs. 11, 17 and after formula for auxiliary functions

$$B_{0,l}^{k}(\beta) = (k-1)\, B_{0,l-1}^{k-1}(\beta) \tag{68}$$

We obtain

$$d_{j,m-1}^{j}(\beta) = \sqrt{\frac{j+m}{j-m+1}}\tan\frac{\beta}{2} d_{j,m}^{j}(\beta) \tag{69}$$

Special values of $d_{m',m}^{j}(\beta)$ are given in terms of $A_{1,1}^{1}(\beta)$ as following forms;

$$\begin{aligned} d_{0,0}^{1}(\beta) &= A_{1,1}^{1}(\beta) - 1 \\ d_{1,0}^{1}(\beta) &= \left\{\frac{1-\left(A_{1,1}^{1}(\beta)-1\right)^{2}}{2}\right\}^{1/2} \\ d_{1,\pm 1}^{1}(\beta) &= \frac{1 \pm \left(A_{1,1}^{1}(\beta)-1\right)}{2} \end{aligned} \tag{70}$$

where $\beta \in [0, \pi)$.

The results for $d_{1,2}^{2}(\beta)$, $d_{2,-2}^{5}(\beta)$, $d_{2,-2}^{5}(\beta)$, and $d_{8,5}^{10}(\beta)$ are shown in Fig. 3. As seen in Fig. 3, $d_{m',m}^{j}(\beta)$ coefficients oscillate but are not periodic. The amplitude of $d_{m',m}^{j}(\beta)$ coefficients isn't constant. $d_{m',m}^{j}(\beta)$ coefficients are equal to $\delta_{m,m'}$ in origin.

5 Implementation and assessment

In the implementation of code, we have used Eqs. 28–45 and 17–20 for $B_{i,l}^{k}(\beta)$ and $A_{m',m}^{j}(\beta)$, respectively. Eq. 11 were used to calculated for finite rotation matrix elements $d_{m',m}^{j}(\beta)$. The program input consist of β angles, highest quantum numbers and initial values of $B_{i,l}^{k}(\beta)$ and $A_{m',m}^{j}(\beta)$.

Using the recurrence relations for $B_{i,l}^{k}(\beta)$ and $A_{m',m}^{j}(\beta)$, we have obtained several numbers recurrence relationships for $d_{m',m}^{j}(\beta)$. Given by Eqs. 53, 56, 65–69 recurrence relationships for $d_{m',m}^{j}(\beta)$ were find literature. Represented by in this study other the recurrence relationships for $d_{m',m}^{j}(\beta)$ are original. The source of originality is auxiliary functions for $d_{m',m}^{j}(\beta)$ (see Eqs. 54, 55, 57–64). Now, one can use our recurrence relationships of $B_{i,l}^{k}(\beta)$ and $A_{m',m}^{j}(\beta)$, other recurrence relationships for $d_{m',m}^{j}(\beta)$ maybe obtained.

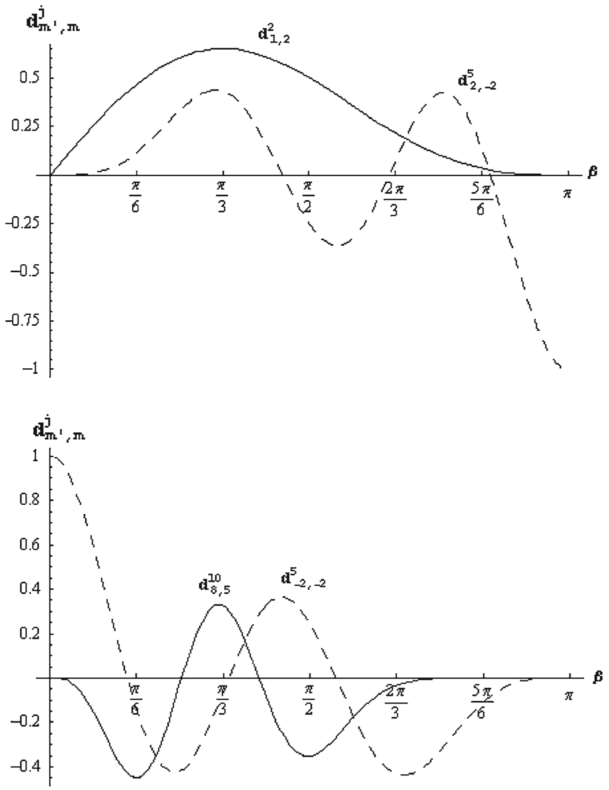

Fig. 3 Finite rotation matrix elements, $d^j_{m',m}(\beta)$, as a function of β and selected values of m, m', and j

The accuracy our program tested by comparing our quantitative results using following orthogonality relationships;

$$\sum_{m=-j}^{j} d^j_{m\sigma}(\beta) d^j_{m\sigma'}(\beta) = \delta_{\sigma\sigma'} \tag{71}$$

$$\sum_{\sigma=-j}^{j} d^j_{m\sigma}(\beta) d^j_{m'\sigma}(\beta) = \delta_{mm'}$$

Those formula are needed only for the test on the accuracy of the rotation matrices. The results found by using recurrence relationships for $B^k_{i,l}(\beta)$ and $A^j_{m',m}(\beta)$, agreed to 18 digit up $j = 150$. The master formulas and values of finite rotation matrix elements $d^j_{m',m}(\beta)$ are presented Table 1 and 2, respectively. As can be seen from Table 2, all calculations were made range $3 \le j \le 150$, $2 \le m' \le 100$, $1 \le m \le 80$, and critical values of β. The results of Table 1 are agreement with Ref. [10]. Same time, as can be seen in Table 1, we have

Table 1 Algebraic expressions for some $d^j_{m',m}(\beta)$ for higher quantum numbers. Symmetry relations may be used in conjunction with this table to evaluate. $x = \cos\beta/2$

j	m'	m	$d^j_{m',m}(\beta)$	j	m'	m	$d^j_{m',m}(\beta)$
3	3	3	x^6	10	10	10	x^{20}
		2	$\sqrt{6}x^5\left(1-x^2\right)^{1/2}$			0	$2\sqrt{46189}x^{10}\left(1-x^2\right)^5$
		1	$\sqrt{15}x^4\left(1-x^2\right)$			−8	$\sqrt{190}x^2\left(1-x^2\right)^9$
		0	$2\sqrt{5}x^3\left(1-x^2\right)^{3/2}$		2	8	$2\sqrt{663}x^{10}\left(1-x^2\right)^3\left(33-114x^2+95x^4\right)$
		−1	$\sqrt{15}x^2\left(1-x^2\right)^2$		0		$\sqrt{24310}x^8\left(1-x^2\right)^4\left(9-38x^2+38x^4\right)$
		−2	$\sqrt{6}x\left(1-x^2\right)^{5/2}$		−6		$\sqrt{102}x^2\left(1-x^2\right)^7\left(3-38x^2+95x^4\right)$
		−3	$\left(1-x^2\right)^3$		−8		$\left(1-x^2\right)^8\left(1-38x^2+190x^4\right)$
5	5	−5	$\left(1-x^2\right)^5$	15	15	15	x^{30}
		−3	$3\sqrt{5}x^2\left(1-x^2\right)^4$			0	$12\sqrt{1077205}x^{15}\left(1-x^2\right)^{15/2}$
		−1	$\sqrt{210}x^4\left(1-x^2\right)^3$			−2	$15\sqrt{532266}x^{13}\left(1-x^2\right)^{17/2}$
	3	3	$x^6\left(28-72x^2+45x^4\right)$		10	15	$-3\sqrt{15834}x^{25}\left(1-x^2\right)^{5/2}$
		1	$\sqrt{42}x^4\left(1-x^2\right)\left(5-18x^2+15x^4\right)$			14	$-3\sqrt{13195}x^{24}\left(1-x^2\right)^2\left(5-6x^2\right)$
		0	$2\sqrt{35}x^3\left(1-x^2\right)^{3/2}\left(2-9x^2+9x^4\right)$			−15	$3\sqrt{15834}x^5\left(1-x^2\right)^{25/2}$
	1	−5	$\sqrt{210}x^4\left(1-x^2\right)^3$	20	20	−15	$6\sqrt{18278}x^5\left(1-x^2\right)^{35/2}$
		4	$2\sqrt{21}x^5\left(3-5x^2\right)\left(1-x^2\right)^{3/2}$			−10	$4\sqrt{52978783}x^{10}\left(1-x^2\right)^{15}$
		3	$\sqrt{42}x^4\left(1-x^2\right)\left(5-18x^2+15x^4\right)$			0	$6\sqrt{3829070245}x^{20}\left(1-x^2\right)^{10}$
8	8	7	$4x^{15}\left(1-x^2\right)^{1/2}$		18	10	$2\sqrt{61129365}x^{28}\left(1-x^2\right)^4\left(29-78x^2+52x^4\right)$
		5	$4\sqrt{35}x^{13}\left(1-x^2\right)^{3/2}$		17		$2\sqrt{2144890}x^{27}\left(1-x^2\right)^{7/2}\left(-406+19x^2\left(87-117x^2+52x^4\right)\right)$

Table 1 continued

j	m'	m	$d^j_{m',m}(\beta)$	j	m'	m	$d^j_{m',m}(\beta)$
		0	$3\sqrt{1430}x^8\left(1-x^2\right)^4$		−20		$4\sqrt{52978783}x^{10}\left(1-x^2\right)^{15}$
	4	8	$2\sqrt{455}x^{12}\left(1-x^2\right)^2$	25	25	20	$14\sqrt{10810}x^{45}\left(1-x^2\right)^{5/2}$
		7	$2\sqrt{455}x^{11}\left(1-x^2\right)^{3/2}\left(3-4x^2\right)$			15	$7\sqrt{209638330}x^{40}\left(1-x^2\right)^5$
		−5	$-2\sqrt{13}x\left(1-x^2\right)^{9/2}\left(1-7x^2\left(3-15x^2+20x^4\right)\right)$			10	$4\sqrt{140676848445}x^{35}\left(1-x^2\right)^{15/2}$
		−8	$2\sqrt{455}x^4\left(1-x^2\right)^6$			0	$42\sqrt{71661341518}x^{25}\left(1-x^2\right)^{25/2}$
	0	3	$2\sqrt{2310}x^3\left(1-x^2\right)^{3/2}$ $\left(1-2x^2\right)\left(1-13x^2+52x^4-78x^6+39x^8\right)$			−12	$70\sqrt{72420514}x^{13}\left(1-x^2\right)^{37/2}$
		−5	$-6\sqrt{2002}x^5\left(1-x^2\right)^{5/2}\left(1-7x^2+15x^4-10x^6\right)$	30	30	30	x^{60}
		−8	$3\sqrt{1430}x^8\left(1-x^2\right)^4$			15	$4\sqrt{3324630574545}x^{45}\left(1-x^2\right)^{15/2}$
	−5	5	$\left(1-x^2\right)^5\left(-1+7x^2\left(6-45x^2+80x^4\right)\right)$			10	$21\sqrt{9505316339695}x^{40}\left(1-x^2\right)^{10}$
		2	$\sqrt{1430}x^3\left(1-x^2\right)^{7/2}\left(2-7x^2\left(3-9x^2+8x^4\right)\right)$		−20	30	$3\sqrt{8377114174}x^{10}\left(1-x^2\right)^{25}$
		−5	$x^{10}\left(-286+7x^2\left(156-195x^2+80x^4\right)\right)$		−30	30	$\left(1-x^2\right)^{30}$

Table 2 Numerical results for $d^{j}_{m',m}(\beta)$

j	m'	m	β	$d^{j}_{m',m}(\beta)$
3	2	1	$\pi/2$	**−0.39528470752104742**
5	4	3	$\pi/2$	**−0.39774756441743298**
6	−3	4	$\pi/3$	**−0.18992194931675325**
9	3	−3	$\pi/2$	**0.22656250000000000**
10	5	10	$\pi/2$	**−0.12159673762713579**
12	12	3	$\pi/2$	**0.27916538371080743**
14	10	10	$\pi/3$	**−0.27914785221219063**
18	8	6	$\pi/3$	**0.04006627746129195**
20	15	17	$\pi/2$	**−0.03043084126805625**
25	−10	5	$\pi/3$	**−0.18931244477432999**
30	20	18	$\pi/2$	**0.02796192362107062**
40	35	10	$\pi/2$	**0.17464470875055721**
50	30	40	$\pi/2$	**0.16401501429205035**
60	50	45	$\pi/3$	**−0.08952565361229781**
80	60	45	$\pi/3$	**0.08917018993502389**
100	20	10	$\pi/3$	**0.08610651631313937**
120	50	40	$\pi/3$	**0.06932286486913012**
150	**100**	**80**	$\pi/3$	**−0.06849087031050788**

$$d^{j}_{j,j}(\beta) = \left(\cos^2 \frac{\beta}{2}\right)^{j} \tag{72}$$

For reference purposes we list in Table 1 for algebraic expressions and Table 2 for numerical calculations the matrix elements of $d^{j}_{m',m}(\beta)$. Explicit expressions for $d^{j}_{m',m}(\beta)$ for $j = 3, 4, 5,$ and 6 may be found elsewhere [11]. We have also compared our results with results of Refs. [12–14]. In this comparison a perfect matching is obtained. Computations with the finite rotation matrix elements of $d^{j}_{-m',m}(\beta)$ or $d^{j}_{m',-m}(\beta)$, we used Eq. 3.

The symmetry properties and special values for auxiliary functions of $B^{k}_{i,l}(\beta)$ and $A^{j}_{m',m}(\beta)$ are taken into account from the calculated $B^{k}_{i,l}(\beta)$ and $A^{j}_{m',m}(\beta)$ and taken into account from stored coefficients. For example, in order to put into, or get it get back from memory the position of certain coefficients $d^{j}_{m',m}(\beta)$ is determined by following relations;

$$f^{j}_{m,m'} = j\left(j^2 + 3j + 2m + 1\right) + \frac{j\,(j-1)\,(j-2)}{3} + m + m' + 1 \tag{73}$$

We confirmed this inference by the additionally calculating the elements to sufficient accuracy using MATHEMATICA [15], recurrence relations, relationships of hypergeometric functions and Jacobi polynomials, and Gauss' recurrence relationships [6].

References

1. A.R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, New Jersey, 1960)
2. U. Fano, G. Racah, *Irreducible Tensorial Sets* (Academic Press, New York, 1957)
3. M.E. Rose, *Elementary Theory of Angular Momentum* (John Wiley, New York, 1967)
4. S.L. Altmann, C.J. Bradley, Philos. Trans. R. Soc. London Ser. A **255**, 193 (1961)
5. G.B. Arfken, H.J. Weber, *Mathematical Methods for Physicists* (Academic Press, Orlando, 2001)
6. I.S. Gradshteyn, I.M. Ryzhik, *Tables of Integrals, Sums, Series and Products* (Academic Press, New York, 1965)
7. J. Pagaran, S. Fritzsche, G. Gaigalas, Comp. Phys. Commun. **174**, 616 (2006)
8. M.A. Blanco, M. Florez, M. Bermejo, J. Mol. Struct. (Theochem) **419**, 19 (1997)
9. S.T. Lai, Y.N. Chio, J. Math. Phys. **30**(4), 844 (1989)
10. R.N. Zare, *Angular Momentum, Understanding Spatial Aspects in Chemistry and Physics* (John Wiley & Sons Inc., New York, 1988)
11. J. Ivanic, K. Ruedenberg, J. Phys. Chem. **100**, 6342 (1996); **102**, 9099 (1998)
12. Y.N. Chiu, J. Chem. Phys. **45**, 2969 (1966)
13. C.H. Choi, J. Ivanic, M.S. Gordon, K. Ruedenberg, J. Chem. Phys. **111**(19), 8825 (1999)
14. J.R.A. Collado, J.F. Rico, R. Lopez, M. Paniagua, G. Ramirez, Comp. Phys. Commun. **52**, 323 (1989)
15. S. Wolfram, *Mathematica, A System for Doing Mathematics by Computer* (Addision Wesley, New York, 1998)