Süleyman Demirel Üniversitesi Fen Edebiyat Fakültesi Fen Dergisi https://dergipark.org.tr/sdufeffd
Süleyman Demirel University Faculty of Arts and Sciences Journal of Science e-ISSN: 1306-7575
Research Article, 2023, 18(3): 213-222, DOI: 10.29233/sdufeffd.1312399

Evaluation of the Gaunt Coefficients by Using Recurrence Relations for Spherical Harmonics

Selda Özay

Department of Physics, Faculty of Science, Ondokuz Mayıs University, 55139, Samsun, TURKEY
https://orcid.org/0000-0001-5205-4519
**corresponding author: seldaozay@hotmail.com*

(Received: 09.06.2023, Accepted: 12.09.2023, Published: 23.11.2023)

Abstract: The Gaunt coefficient is one of the important coefficients to be known for calculating molecular integrals in quantum theory of coupling of three angular momenta. Generally, these coefficients are calculated analytically by using the properties of the associated Legendre polynomials. In this study, Gaunt coefficients were calculated algebraically by using the recurrence relations and orthogonality conditions of spherical harmonics and different mathematical expressions were obtained from known analytical expressions for Gaunt coefficients in terms of factorial functions or binomial coefficients. By using the program written in the Mathematica programming language, both the analytical expressions and the algebraic expressions were calculated, and the numerical results obtained were compared. Numerical results are in quite agreement with the literature and each other.

Key words: Clebsch – Gordan coefficients, Vector coupling coefficients, Gaunt coefficients.

1. Introduction

Since atoms and molecules are quantum mechanical systems, in order to study their electronic structure, physical and chemical properties, the Hamiltonian operator of the system must be written, and the Schrödinger equation of the system must be solved. The repulsive Coulomb potential energy term between electrons in atoms and molecules depends on the distances between two electrons and is inversely proportional to the distance term dependent on the coordinates of both electrons. Therefore, this interaction term between electrons cannot be written separately depending on the coordinates of individually electrons. This makes it impossible to solve the Schrödinger equation analytically for multi-electron systems without using approximate methods. It should be known that there is no mathematical difficulty in single-electron systems. The most suitable coordinate system to solve the Schrödinger equation in such systems is spherical coordinates. If spherical coordinates are used, the kinetic energy operators of individual particles are written as

$$T = -\frac{\hbar^2}{2\,m}\left\{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{L^2}{\hbar^2\,r^2}\right\} \tag{1}$$

the form of the square of the angular momentum operator.

In central field problems, since the Hamiltonian operator of the system commute with the square of the angular momentum and the component z of the angular momentum. The spherical harmonics are the eigenfunctions of L^2 and also the eigenfunctions of the Hamiltonian operator. Therefore, the angular part of the spatial wave functions of all atoms and molecules is composed of spherical harmonics.

Spherical harmonics are given by associated Legendre polynomials, P_l^m, as follows [1]

$$Y_l^m(\theta,\phi) = (-1)^m \sqrt{\frac{2\,l+1}{4\pi}\,\frac{(l-m)\,!}{(l+m)\,!}}\; P_l^m(cos\theta)\, e^{i\,m\,\phi}\,, \qquad m \geq 0 \tag{2.a}$$

Spherical harmonics for negative superscript is given by

$$Y_l^{-|m|}(\theta,\phi) = (-1)^m \left[Y_l^{|m|}(\theta,\phi)\right]^* \tag{2.b}$$

Spherical harmonics have a very wide range of applications not only in atomic and molecular physics, but also in solid-state physics, nuclear physics, astrophysics, and many areas of chemistry.

In the second part of this study, functions consisting of the product of spherical harmonics and trigonometric functions are written again in terms of spherical harmonics. In the third part, the Gaunt coefficients are calculated algebraically using the integral expression for the Gaunt coefficients and the recurrence relations of the spherical harmonics in the second part. The numerical results of the obtained mathematical expression are calculated with the Mathematica program, the results are presented as Table 1 in the fourth part. The accuracy of the results found was checked using the orthogonality relation and compared with the literature.

2. Material and Method

2.1. Recurrence relations for spherical harmonics

In multipole moment transitions that occur as a result of the interaction of atoms with the external electric and magnetic fields, the products of one spherical harmonic and trigonometric function (or product of trigonometric and exponential function) emerge. To calculate multipole moment integrals, it is possible to write recurrence relations for spherical harmonics using the recurrence relations provided by the associated Legendre polynomials. Some of these relations are given below [1, 2].

$$cos\theta\, Y_L^M(\theta,\phi) = \sqrt{\frac{(L-M+1)(L+M+1)}{(2L+1)(2L+3)}}\; Y_{L+1}^M + \sqrt{\frac{(L-M)(L+M)}{(2L-1)(2L+1)}}\; Y_{L-1}^M \tag{3}$$

$$sin\theta\, Y_L^M(\theta,\phi)\, e^{i\,\phi} = -\sqrt{\frac{(L+M+1)(L+M+2)}{(2L+1)(2L+3)}}\; Y_{L+1}^{M+1} + \sqrt{\frac{(L-M-1)(L-M)}{(2L-1)(2L+1)}}\; Y_{L-1}^{M+1} \tag{4}$$

$$sin\theta\, Y_L^M(\theta,\phi)\, e^{-i\,\phi} = \sqrt{\frac{(L-M+1)(L-M+2)}{(2L+1)(2L+3)}}\; Y_{L+1}^{M-1} - \sqrt{\frac{(L+M-1)(L+M)}{(2L-1)(2L+1)}}\; Y_{L-1}^{M-1} \tag{5}$$

$$\begin{aligned}(2L-1)(2L+3)\cos^2\theta\, Y_L^M(\theta,\phi) = {}& (2l-1)\sqrt{\frac{((L+1)^2-M^2)((L+2)^2-M^2)}{(2L+1)(2L+5)}}\; Y_{L+2}^M \\ & +[2L(L+1)-2M^2-1]\, Y_L^M \\ & +(2l+3)\sqrt{\frac{(L^2-M^2)((L-1)^2-M^2)}{(2L+1)(2L-3)}}\; Y_{L-2}^M\end{aligned} \tag{6}$$

$$(2L-1)(2L+3)\; sin\theta\;\cos\theta\, e^{i\phi}\, Y_L^M(\theta,\phi) =$$

$$-(2l-1)\sqrt{\frac{((L+1)^2-M^2)(L+M+2)(L+M+3)}{(2L+1)(2L+5)}}\;Y_{L+2}^{M+1}$$
$$-(2M+1)\sqrt{L(L+1)-M(M+1)}\;Y_L^{M+1} \quad (7)$$
$$+(2l+3)\sqrt{\frac{(L^2-M^2)(L-M-1)(L-M-2)}{(2L+1)(2L-3)}}\;Y_{L-2}^{M+1}$$

$$(2L-1)(2L+3)\,sin\theta\;\cos\theta\,e^{-i\phi}\,Y_L^M(\theta,\phi) =$$
$$(2L-1)\sqrt{\frac{((L+1)^2-M^2)(L-M+2)(L-M+3)}{(2L+1)(2L+5)}}\;Y_{L+2}^{M-1}$$
$$-(2M-1)\sqrt{L(L+1)-M(M-1)}\;Y_L^{M-1} \quad (8)$$
$$-(2l+3)\sqrt{\frac{(L^2-M^2)(L+M-1)(L+M-2)}{(2L+1)(2L-3)}}\;Y_{L-2}^{M-1}$$

$$(2L-1)(2L+3)\;\sin^2\theta\;\,e^{2i\phi}\,Y_L^M(\theta,\phi) =$$
$$\frac{2L-1}{\sqrt{(2L+1)(2L+5)}}\sqrt{\frac{(L+M+4)!}{(L+M)!}}\;Y_{L+2}^{M+2}$$
$$+\frac{2L+3}{\sqrt{(2L+1)(2L-3)}}\sqrt{\frac{(L-M)!}{(L-M-4)!}}\;Y_{L-2}^{M+2} \quad (9)$$
$$-2\sqrt{\frac{(L+M+2)!(L-M)!}{(L-M-2)!(L+M)!}}\;Y_L^{M+2}$$

$$(2L-1)(2L+3)\;\sin^2\theta\;\,e^{-2i\phi}\,Y_L^M(\theta,\phi) =$$
$$\frac{2L-1}{\sqrt{(2L+1)(2L+5)}}\sqrt{\frac{(L-M+4)!}{(L-M)!}}\;Y_{L+2}^{M-2}$$
$$+\frac{2L+3}{\sqrt{(2L+1)(2L-3)}}\sqrt{\frac{(L+M)!}{(L+M-4)!}}\;Y_{L-2}^{M-2} \quad (10)$$
$$-2\sqrt{\frac{(L-M+2)!(L+M)!}{(L+M-2)!(L-M)!}}\;Y_L^{M-2}$$

In many-particle systems, the total angular momentum of the system is composed of the vector sum of the orbital angular momenta of the particles. The situation is a bit more complicated in atoms and molecules. Because, in addition to the orbital angular momenta of the electrons, there are also spin angular momenta that are independent of the orbital motion. In atoms and molecules, the total angular momentum which is expressed of the sum of these two angular momenta, needs to be investigated. ***H*** Hamiltonian operator of the system commutes with L^2, S^2, L_z and S_z so that these are constants of motion and corresponding quantum numbers l, s, m_l and m_s are all *good quantum numbers*. It is possible to write the wave function of the system that is composed of the individual wave functions of the electrons (superposition principle). In this case, the linear combination coefficients are called Clebsch – Gordan coefficients [2] and are defined in terms of $F(a,b)$ binomial coefficients [3] as follows.

$$C^{L\,M}_{l_1m_1,l_2m_2} = \langle l_1m_1\, l_2m_2|l_1l_2LM\rangle = \langle l_1l_2LM|l_1m_1\, l_2m_2\rangle$$

$$= \delta_{M,m_1+m_2}\left[\frac{F(2l_1,l_1+l_2-L)\,F(2l_2,l_1+l_2-L)}{F(l_1+l_2+L+1,l_1+l_2-L)F(2l_1,l_1-m_1)F(2l_2,l_2-m_2)F(2L,L-M)}\right]^{1/2} \quad (11)$$

$$\sum_z\{(-1)^z F(l_1+l_2-L,z)$$

$$F(l_1-l_2+L,l_1-m_1-z)F(-l_1+l_2+L,l_2+m_2-z)\}$$

where the summation index z is described in Refs. [2, 3].

To calculate the Clebsch – Gordan coefficients, the raising/lowering operators of the angular momentum operators are used. This is quite laborious task for high quantum numbers. In the use of computers, there is a problem of memory stacking. Clebsch – Gordan coefficients have been calculated analytically by many researchers using analytical methods, and the results are generally given in terms of factorial functions or binomial coefficients [4-12].

Clebsch – Gordan coefficients are the most general coefficients related to rotational motion. Therefore, all other coefficients related to rotation are written in terms of Clebsch – Gordan coefficients. One of these rotation coefficients is the Gaunt coefficient. Gaunt coefficients are defined as the product of three spherical harmonics by following form in terms of Clebsch – Gordan coefficients [13-19].

For $\Delta M = m_1 - m_2$

$$Y^{L\,M}_{l_1m_1,l_2m_2} = \int_0^{2\pi}\int_0^{\pi}\left(Y^{m_1}_{l_1}\right)^* Y^{m_2}_{l_2}\, Y^M_L\, sin\theta\, d\theta\, d\phi \quad (12)$$

$$= (-1)^{m_2}\sqrt{\frac{(2\,l_1+1)\,(2\,l_2+1)}{4\,\pi\,(2L+1)}}\; C^{L0}_{l_10,l_20}C^{LM}_{l_1m_1,l_2-m_2}$$

and for $\Delta M = m_1 + m_2$

$$Y^{L\,M}_{l_1m_1,l_2m_2} = \int_0^{2\pi}\int_0^{\pi} Y^{m_1}_{l_1}\, Y^{m_2}_{l_2}\, (Y^M_L)^*\, sin\theta\, d\theta\, d\phi \quad (13)$$

$$= \sqrt{\frac{(2\,l_1+1)\,(2\,l_2+1)}{4\,\pi\,(2L+1)}}\; C^{L0}_{l_10,l_20}C^{LM}_{l_1m_1,l_2m_2}$$

Using the Clebsch – Gordan coefficients given in Refs. [5, 7, 20] in terms of factorial and binomial coefficients and Eqs. (12, 13), the Gaunt coefficients are written in terms of generalized hypergeometric functions whose argument is equal to 1 [21].

$$Y^{L\,M}_{l_1m_1,l_2m_2} = (-1)^{\frac{3l_1+l_2-L-2m_1}{2}}\left(\frac{1+(-1)^{l_1+l_2+L}}{2}\right)\sqrt{\frac{(2l_1+1)(2l_2+1)(2L+1)}{4\pi}}$$

(14)

$$\frac{F\left(l_2,\frac{l_2+L-l_1}{2}\right) F\left(\frac{l_1+l_2+L}{2}, l_2\right) F(l_2+L-m_1,l_2-L+m_1)}{(l_1+l_2+L+1)\, F(2L,2m_1)}$$

$$\sqrt{\frac{F(-l_1+l_2+L,L)\, F(2L,l_1-l_2+L)\, F(L+M,L-M)\, F(2m_1+2m_2,2m_1)}{F(l_1+l_2+L,2L)\, F(2L,L)\, F(L,l_2-l_1)\, F(l_1+l_2+L,2L)\, F(l_2+m_2,l_2-m_2)}}$$

$${}_3F_2\left[\begin{matrix} l_1+m_1+1, -l_1+\ m_1, -L+M \\ -l_1-L+m_1,\ l_2-\ L+\ m_1+1 \end{matrix}\middle| 1\right]$$

In this study, Gaunt coefficients were calculated algebraically using the recurrence relations of spherical harmonics and numerical values were obtained by using the Mathematica programming language [22].

2.2. Gaunt coefficients

According to Eq. (12 or 13), the expansion of spherical harmonics given by Eq. (2) should be used to calculate the Gaunt coefficients analytically. Since the double integral over a sphere (both θ and ϕ limits are constant) is product, the Gaunt coefficients are written as the product of two independent integrals. While it is difficult to calculate integrals via the associated Legendre polynomials, it is quite easy to calculate the integral via the azimuthal angle which gives the necessary selection rules for the Gaunt coefficients to be nonzero. The selection rules are $\Delta M = m_1 \pm m_2$ according to the spherical harmonic chosen as the complex. If the Gaunt coefficients are calculated using the Eqs. (12-14), these selection rules must be taken into account. Because, when the condition $\Delta M = m_1 - m_2$ is satisfied, the Gaunt coefficient is different from zero but the Clebsch – Gordan coefficient becomes zero unless $m_2 = -m_2$ in the expressions for the Clebsch – Gordan coefficient.

When algebraic methods will be used instead of analytical methods to calculate the Gaunt coefficients, recurrence and orthogonality relations of spherical harmonics given by Eqs. (3-10) will be used. For $l_2 = 1$ and $m_2 = 0$, if special values of spherical harmonics for this quantum sets is used, Eq. (12) rewritten as follows

$$Y_{l_1 m_1,10}^{L\,M} = \sqrt{\frac{3}{4\pi}} \int_0^{2\pi} \int_0^{\pi} \left(Y_{l_1}^{m_1}\right)^* (\cos\theta\, Y_L^M)\, \sin\theta\, d\theta\, d\phi$$

In this equation, if the recurrence relation given by Eq. (3) is replaced with the product of trigonometric function and spherical harmonics, the orthogonality relation of spherical harmonics is used in the integral expression and then obtained.

$$Y_{l_1 m_1,10}^{LM} = \sqrt{3}\left\{\sqrt{\frac{(L-M+1)(L+M+1)}{(2L+1)(2L+3)}}\, Y_{l_1 m_1,00}^{L+1 M} + \sqrt{\frac{(L-M)(L+M)}{(2L-1)(2L+1)}}\, Y_{l_1 m_1,00}^{L-1 M}\right\} \tag{15}$$

In order to calculate the $Y_{l_1 m_1,10}^{LM}$ Gaunt coefficients, it is sufficient to give only L and M quantum numbers to this obtained equation.

By changing the values of the l_2 and m_2 quantum numbers and repeating the above operations, the Gaunt coefficients for different quantum sets can be obtained as follows:

$$Y_{l_1 m_1,11}^{LM} = \sqrt{3/2}\left\{\sqrt{\frac{(L+M+1)(L+M+2)}{(2L+1)(2L+3)}}\, Y_{l_1 m_1,00}^{L+1 M+1} - \sqrt{\frac{(L-M)(L-M-1)}{(2L-1)(2L+1)}}\, Y_{l_1 m_1,00}^{L-1 M+1}\right\} \tag{16}$$

(17)

$$Y^{LM}_{l_1m_1,1-1} = \sqrt{3/2}\left\{\sqrt{\frac{(L-M+1)(L-M+2)}{(2L+1)(2L+3)}}\ Y^{L+1M-1}_{l_1m_1,00} - \sqrt{\frac{(L+M)(L+M-1)}{(2L-1)(2L+1)}}\ Y^{L-1M-1}_{l_1m_1,00}\right\}$$

$$Y^{LM}_{l_1m_1,20} = \sqrt{5}\left\{\frac{3}{2(2L-1)(2L+3)}\left[(2L-1)\sqrt{\frac{((L+1)^2-M^2)((L+2)^2-M^2)}{(2L+1)(2L+5)}}\ Y^{L+2M}_{l_1m_1,00}\right.\right.$$
$$+(2L(L+1)-2M^2-1)\ Y^{LM}_{l_1m_1,00} \tag{18}$$
$$\left.\left.+(2L+3)\sqrt{\frac{(L^2-M^2)((L-1)^2-M^2)}{(2L+1)(2L-3)}}\ Y^{L-2M}_{l_1m_1,00}\right] - \frac{1}{2}\ Y^{LM}_{l_1m_1,00}\right\}$$

$$Y^{LM}_{l_1m_1,21} = 3\sqrt{\frac{5}{6}}\left\{\frac{1}{(2L-1)(2L+3)}\left[(2L-1)\sqrt{\frac{((L+1)^2-M^2)(L+M+2)(L+M+3)}{(2L+1)(2L+5)}}\ Y^{L+2M+1}_{l_1m_1,00}\right.\right.$$
$$+(2M+1)\sqrt{L(L+1)-M(M+1)}\ Y^{LM+1}_{l_1m_1,00} \tag{19}$$
$$\left.\left.-(2L+3)\sqrt{\frac{(L^2-M^2)(L-M-1)(L-M-2)}{(2L+1)(2L-3)}}\ Y^{L-2M+1}_{l_1m_1,00}\right]\right\}$$

$$Y^{LM}_{l_1m_1,2-1} = 3\sqrt{\frac{5}{6}}\left\{\frac{1}{(2L-1)(2L+3)}\left[(2L-1)\sqrt{\frac{((L+1)^2-M^2)(L-M+2)(L-M+3)}{(2L+1)(2L+5)}}\ Y^{L+2M-1}_{l_1m_1,00}\right.\right.$$
$$-(2M-1)\sqrt{L(L+1)-M(M-1)}\ Y^{LM-1}_{l_1m_1,00} \tag{20}$$
$$\left.\left.-(2L+3)\sqrt{\frac{(L^2-M^2)(L+M-1)(L+M-2)}{(2L+1)(2L-3)}}\ Y^{L-2M-1}_{l_1m_1,00}\right]\right\}$$

$$Y^{LM}_{l_1m_1,22} = 3\sqrt{\frac{5}{24}}\left\{\frac{1}{(2L-1)(2L+3)}\left[\frac{2L-1}{\sqrt{(2L+1)(2L+5)}}\sqrt{\frac{(L+M+4)!}{(L+M)!}}\ Y^{L+2M+2}_{l_1m_1,00}\right.\right.$$
$$+\frac{2L+3}{\sqrt{(2L+1)(2L-3)}}\sqrt{\frac{(L-M)!}{(L-M-4)!}}\ Y^{L-2M+2}_{l_1m_1,00} \tag{21}$$
$$\left.\left.-2\sqrt{\frac{(L+M+2)!(L-M)!}{(L-M-2)!(L+M)!}}\ Y^{LM+2}_{l_1m_1,00}\right]\right\}$$

$$Y^{LM}_{l_1m_1,2-2} = 3\sqrt{\frac{5}{24}}\left\{\frac{1}{(2L-1)(2L+3)}\left[\frac{2L-1}{\sqrt{(2L+1)(2L+5)}}\sqrt{\frac{(L-M+4)!}{(L-M)!}}\ Y^{L+2M-2}_{l_1m_1,00}\right.\right.$$
$$+\frac{2L+3}{\sqrt{(2L+1)(2L-3)}}\sqrt{\frac{(L+M)!}{(L+M-4)!}}\ Y^{L-2M-2}_{l_1m_1,00} \tag{22}$$
$$\left.\left.-2\sqrt{\frac{(L-M+2)!(L+M)!}{(L+M-2)!(L-M)!}}\ Y^{LM-2}_{l_1m_1,00}\right]\right\}$$

All Gaunt coefficients given by the Eqs. (15-22) are expressed in terms of the basic Gaunt coefficient defined as

$$Y_{l_1 m_1,00}^{LM} = \frac{1}{\sqrt{4\pi}} \delta_{l_1,L} \delta_{m_1,M} \tag{23}$$

3. Results

As can be seen from the Eqs. (15-22), it is possible to find the Gaunt coefficients numerically according to the given quantum sets by calculating the multipliers of the basic Gaunt coefficients. Given Eqs. (14 and 15-22) Gaunt coefficients were calculated by algorithm written in Mathematica programming language based on these formulas and the results are given in Table 1. The numerical values given in Table 1 are in agreement with Refs. [15, 16, 19 and 23].

Written program by using Eqs. (14 and 15-22) are run on Intel (R) Core (TM) i5-6200U CPU @ 2.30 Ghz computer for some sets of quantum numbers and the CPU times are found, and the results are given in seconds in Table 2. Since the computers used have different hardware, the CPU times are not compared with the literature.

Table 1. Gaunt coefficients for different sets of quantum numbers by using Eqs. (15-22 and 14).

l_1	m_1	l_2	m_2	l	m	$\frac{1}{\sqrt{\pi}}$ Eqs. (15-22)	Eq. (14)
10	5	0	0	10	5	1/2	0.2820947917738781
15	8	1	0	14	8	$\frac{1}{2}\sqrt{483/899}$	0.2067705997734994
25	-8	1	0	26	-8	$3/\sqrt{53}$	0.2324921981102874
20	13	1	1	19	12	$2\sqrt{33/533}$	0.2807685277668304
30	-15	1	1	31	-16	$-\frac{1}{2}\sqrt{1081/1281}$	−0.2591393410513699
40	18	1	-1	39	19	$\frac{1}{6}\sqrt{77/79}$	0.09283369360381252
15	5	1	-1	16	6	$-\frac{1}{2}\sqrt{21/31}$	−0.2321794983075630
12	6	2	0	10	6	$\frac{9}{46}\sqrt{17/7}$	0.1720224711335037
14	7	2	0	14	7	$\frac{7\sqrt{5}}{186}$	0.04747830014554065
6	5	2	0	8	5	$\frac{3}{\sqrt{170}}$	0.1298140972960522
64	50	2	1	62	49	$\frac{14}{635}\sqrt{12882/43}$	0.2152964127263299
8	4	2	1	8	3	$\frac{7}{19\sqrt{2}}$	0.1469787348847384
12	7	2	1	14	6	$-\frac{2}{9}\sqrt{14/19}$	−0.08711191655125597
38	15	2	-1	36	16	$\frac{1}{10}\sqrt{1219/365}$	0.1031051798730726
53	9	2	-1	53	10	$-\frac{19}{109}\sqrt{33/70}$	−0.06752430402507384

45	18	2	-1	47	19	$-\frac{8}{31}\sqrt{55/19}$	-0.2477181917039297
79	24	2	2	77	22	$\frac{5}{314}\sqrt{530553/1643}$	0.1614399541279544
83	65	2	2	85	63	$\frac{5}{338}\sqrt{77/167}$	0.005667160268083574
34	27	2	2	34	25	$-\frac{90\sqrt{61}}{4757}$	-0.08336799160917377
49	5	2	-2	47	7	$\frac{1}{194}\sqrt{12341/19}$	0.07411766167839542
24	9	2	-2	26	11	$\frac{5}{2}\sqrt{111/6307}$	0.1871178187511329
96	47	2	-2	96	49	$-\frac{84\sqrt{58}}{2483}$	-0.1453588997129646

Table 2. Computational times for some sets of quantum numbers in Table 1.

l_1	m_1	l_2	m_2	l	m	CPU (in seconds)	
						Eqs. (15-22)	Eq.(14)
10	5	0	0	10	5	0.234	0.266
30	-15	1	1	31	-16	0.296	0.218
64	50	2	1	62	49	0.328	0.282
53	9	2	-1	53	10	0.329	0.328
83	65	2	2	85	63	0.297	0.344
96	47	2	-2	96	49	0.266	0.329

4. Conclusion

To check the accuracy of the obtained numerical results, we used orthogonality relation for the Gaunt coefficients provided by following form [23]

$$\sum_{m_1=-l_1}^{l_1}\sum_{m_2=-l_2}^{l_2} Y_{l_1m_1,l_2m_2}^{L\,M} Y_{l_1m_1,l_2m_2}^{L'\,M'} = Y_{l_10,l_20}^{L\,0}\sqrt{\frac{(2\,l_1+1)\,(2\,l_2+1)}{4\,\pi\,(2L+1)}}\,\delta_{L,L'}\delta_{M,M'} \qquad (24)$$

Since the m_2 value is constant in the Eqs. (15-22), it is sufficient to add only summation via m_1 instead of the two sums in the orthogonality relation.

In this study, the advantage of the formulas obtained for the Gaunt coefficients is that they are valid when both selection rules of the form $\Delta M = m_1 \pm m_2$ are satisfied.

Authorship contribution statement

S. Özay: Conceptualization, Methodology, Software, Validation, Investigation, Original Draft Writing, Review and Editing.

Declaration of competing interest

The author declares that I have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgment

As the author of this study, I declare that I do not have any support and thank you statement.

Ethics Committee Approval and/or Informed Consent Information

As the author of this study, I declare that I do not have any ethics committee approval and/or informed consent statement.

References

[1] G. B. Arfken and H. J. Weber, Mathematical Methods for Physicists, 4th ed., London, Academic Press, 1029 pages, 2001.
[2] D. A. Varshalovich, A. N. Moskalev and V. K. Khersonskii, Quantum Theory of Angular Momentum, Irreducible Tensors, Spherical Harmonics, Vector Coupling Coefficients, *3nj* Symbols, Singapore, World Scientific Publishing Co. Pte. Ltd, 514 pages, 1988.
[3] T. Shimpuku, "General Theory and Numerical Tables of Clebsch-Gordan Coefficients", *Progress of Theoretical Physics Supplement*, 13, 1-136, 1960.
[4] A. Bandzaitis and A. Yutsis, "Once more on the formulas for the Clebsch-Gordan coefficients", Lietuvos Fiz. Rinkinys, 4, 45-49, 1964.
[5] V. A. Fock, "New deduction of the vector model", JETP 10, 383-393, 1940.
[6] S. D. Majumdar, "The Clebsch-Gordan coefficients", *Progress of Theoretical Physics*, 20(6), 798-803, 1958.
[7] G. Racah, "Theory of complex spectra. II", *Physical Review*, 62(9), 438-462, 1942.
[8] A. R. Edmonds, Angular Momentum in Quantum Mechanics, 2nd ed., New Jersey, Princeton University Press, 146 pages, 1960.
[9] M. E. Rose, Elementary Theory of Angular Momentum, New York, John Wiley&Sons, 248 pages, 1957.
[10] R. N. Zare, Angular Momentum, Understanding Spatial Aspects in Chemistry and Physics, New York, John Wiley&Sons, 349 pages, 1988.
[11] E. U. Condon and G. H. Shortley, The Theory of Atomic Spectra, Cambridge, Cambridge University Press, 441 pages, 1959.
[12] A. R. Edmonds, Angular Momenta in Quantum Mechanics, CERN 55-26, Geneva, 82 pages, 1955.
[13] J. A. Gaunt, "The triplets of Helium", *Philosophical Transactions of the Royal Society of London Series A*, 228, 151-196, 1929.
[14] O. R. Cruzan, "Translational addition theorems for spherical vector wave functions", Quarterly Applied Mathematics, 20, 33-40, 1962.
[15] Y. L. Xu, "Fast evaluation of Gaunt coefficients", *Mathematics of Computation*, 65(216), 1601-1612, 1996.
[16] E. J. Weniger and E. O. Steinborn, "Programs for the coupling of spherical harmonics, *Computer Physics Communications*, 25, 149-157, 1982.
[17] J. Rasch and A. C. H. Yu, "Efficient storage scheme for precalculated Wigner 3j, 6j and Gaunt coefficients", *Journal on Scientific Computing*, 25(4), 1416-1428, 2004.
[18] H. H. Homeier and E. O. Steinborn, "Some properties of the coupling coefficients of real spherical harmonics and their relation to Gaunt coefficients", *Journal of Molecular Structure (Theochem)*, 368, 31-37, 1996.
[19] S. A. Yükçü, N. Yükçü and E. Öztekin, "New representations for Gaunt coefficients", *Chemical Physics Letters*, 735 (UNSP 136769), 1-3, 2019.
[20] E. P. Wigner, Group Theory, New York, Academic Press, 372 pages, 1959.
[21] E. L. Akim and A. A. Levin, "Generating Function for Clebsch-Gordan Coefficients", *Doklady Akademii Nauk USSR*, 138, 503-505, 1961.

[22] S. Wolfram, A system for doing mathematics by computer, 2nd ed., United Kingdom, Addison Wesley, 261 pages, 1998.
[23] D. Sebilleau, "On the computation of the integrated products of three spherical harmonics", *Journal of Physics A: Mathematical and General Physics*, 31(34), 7157-7168, 1998.