Author(s) : K.S. Kölbig **Library:** MATHLIB
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Wigner 3-j, 6-j, 9-j Symbols; Clebsch-Gordan, Racah W-, Jahn U-Coefficients

Function subprograms `RWIG3J`, `DWIG3J`; `RWIG6J`, `DWIG6J`; `RWIG9J`, `DWIG9J`; `RCLEBG`, `DCLEBG`; `RRACAW`, `DRACAW` and `RJAHNU`, `DJAHNU` calculate the Wigner 3-j, 6-j and 9-j symbols, the Clebsch-Gordan coefficients, the Racah W-coefficients and the Jahn U-coefficients, respectively.
On CDC and Cray computers, the double-precision versions `DWIG3J` etc. are not available.

Structure:

`FUNCTION` subprograms
User Entry Names: `RWIG3J`, `RWIG6J`, `RWIG9J`, `RCLEBG`, `RRACAW`, `RJAHNU`
`DWIG3J`, `DWIG6J`, `DWIG9J`, `DCLEBG`, `DRACAW`, `DJAHNU`

Usage:

In any arithmetic expression, for `t` $=$ `R` (type `REAL`), or `t` $=$ `D` (type `DOUBLE PRECISION`),

`tWIG3J(A,B,C,X,Y,Z)` has the value of $\begin{pmatrix} a & b & c \\ x & y & z \end{pmatrix}$;

`tWIG6J(A,B,C,X,Y,Z)` has the value of $\begin{Bmatrix} a & b & c \\ x & y & z \end{Bmatrix}$;

`tWIG9J(A,B,C,P,Q,R,X,Y,Z)` has the value of $\begin{Bmatrix} a & b & c \\ p & q & r \\ x & y & z \end{Bmatrix}$;

`tCLEBG(A,B,C,X,Y,Z)` has the value of $(a\,b\,x\,y\,|\,a\,b\,c\,z)$;

`tRACAW(A,B,C,D,E,F)` has the value of $W(a\,b\,c\,d\,;\,e\,f)$;

`tJAHNU(A,B,C,D,E,F)` has the value of $U(a\,b\,c\,d\,;\,e\,f)$.

All the arguments must have integral or half-integral values (see **Notes**). They have the same type as the function name. For definitions and notations see **References**.
The following relations hold (see Refs. 1 and 3):
Clebsch-Gordan coefficient (in terms of the Wigner 3-j symbol):

$$(a\,b\,x\,y\,|\,a\,b\,c\,z) = (-1)^{a-b-z}\sqrt{2c+1}\begin{pmatrix} a & b & c \\ x & y & -z \end{pmatrix};$$

Racah W-coefficient (in terms of the Wigner 6-j symbol):

$$W(a\,b\,c\,d\,;\,e\,f) = (-1)^{a+b+c+d}\begin{Bmatrix} a & b & e \\ d & c & f \end{Bmatrix}.$$

Jahn U-coefficient (in terms of the Wigner 6-j symbol and the Racah W-coefficient):

$$\begin{aligned} U(a\,b\,c\,d\,;\,e\,f) &= (-1)^{a+b+c+d}\sqrt{(2e+1)(2f+1)}\begin{Bmatrix} a & b & e \\ d & c & f \end{Bmatrix} \\ &= \sqrt{(2e+1)(2f+1)}\,W(a\,b\,c\,d\,;\,e\,f). \end{aligned}$$

Method:

The Wigner 3-j symbol and the Clebsch-Gordan coefficient are calculated from formulas (5.1) and (5.10) of Ref. 1, respectively. The Wigner 6-j symbol, the Racah W- and the Jahn U-coefficient are calculated from formulas (5.23) and (5.24) of Ref. 1. In both cases, the factorials are replaced by their logarithms during the calculation. The Wigner 9-j symbol is calculated from formula (5.37) of Ref. 1 in terms of Wigner 6-j symbols.

Notes:

A Wigner-3j symbol $\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$ is considered to be zero unless simultaneously

(i) j_i and m_i have both either integral or half-integral values (each i),

(ii) $j_i \geq |m_i| \geq 0$ (each i),

(iii) $m_1 + m_2 + m_3 = 0$,

(iv) $j_1 - j_2 - m_3$ is an integer,

(v) $j_1 + j_2 + j_3$ is an integer and $j_1 + j_2 \geq j_3, \quad j_2 + j_3 \geq j_1, \quad j_3 + j_1 \geq j_2.$

The conditions (v) are often denoted by $\delta(j_1\, j_2\, j_3)$ and are called the *triangle relations*.

For a Clebsch-Gordan coefficient $(j_1\, j_2\, m_1\, m_2 \,|\, j_1\, j_2\, j_3\, m_3)$, condition (iii) reads $m_1 + m_2 = m_3$ and condition (iv) disappears.

A Wigner-6j symbol $\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix}$ is considered to be zero unless simultaneously

(i) all j_i and l_i have non-negative integral or half-integral values,

(ii) the four *triangle relations* $\delta(j_1\, j_2\, j_3), \quad \delta(j_1\, l_2\, l_3), \quad \delta(l_1\, j_2\, l_3), \quad \delta(l_1\, l_2\, j_3)$ hold.

A Wigner-9j symbol $\begin{Bmatrix} j_{11} & j_{12} & j_{13} \\ j_{21} & j_{22} & j_{23} \\ j_{31} & j_{32} & j_{33} \end{Bmatrix}$ is considered to be zero unless simultaneously

(i) all j_{ik} have non-negative integral or half-integral values,

(ii) the arguments in each row and in each column satisfy the *triangle relations*.

Restrictions:

The sum of arguments in any *triangle relation* must not exceed 100. No test is made.

References:

1. R.D. Cowan, The theory of atomic structure and spectra, (Univ. of California Press, Berkeley CA 1981).
2. A.F. Nikiforov, V.B. Uvarov and Yu.L. Levitan, Tables of Racah coefficients (Pergamon Press, Oxford 1965).
3. M. Rotenberg, R. Bivins, N. Metropolis and J.K. Wooten, Jr., The 3-j and 6-j symbols (Crosby Lockwood, London 1959).
4. D.A. Varshalovich, A.N. Moskalev and V.K. Khersonskii, Quantum theory of angular momentum (World Scientific, Singapore 1988).

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