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COMPUTATION OF BRODY-MOSHINSKY BRACKETS

A. LEJEUNE *
International Centre for Theoretical Physics, P.O. Box 586, Miramare, 34100 Trieste, Italy

and

J. P. JEUKENNE
Theoretical Nuclear Physics, University of Liège, Sart Tilman, 4000 Liège 1, Belgium

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PROGRAM SUMMARY

Title of program (32 characters maximum): BRODY-MOSHINSKY BRACKETS

Catalogue number: ABGC

Computer for which the program is designed and others upon which it is operable

Computer: IBM 360/65. *Installation*: University of Liège

Operating system or monitor under which the program is executed: OS 360

Programming languages used: FORTRAN IV(G)

High speed store required: 8130 words. *No. of bits in a word*: 64

Is the program overlaid? No

No. of magnetic tapes required: None

What other peripherals are used? Card Reader; Line Printer

No. of cards in combined program and test deck: 579

Card punching code: BCD (026)

CPC Library subprograms used
Catalogue number: ABMA; *Title*: RACAH; *Ref. in CPC*: 1 (1970) 337

Keywords descriptive of problem and method of solution: Nuclear, Nuclear Spectra, Nuclear Structure, Two-Body Operator Matrix Elements, Hartree-Fock Calculations, Brody-Moshinsky Brackets.

Nature of the physical problem
The program computes the Brody-Moshinsky brackets $\langle nl, NL, \lambda | n_1 l_1, n_2 l_2, \lambda \rangle$ defined in refs. [1,2] and appearing in the calculation of matrix elements of two-body operators, when the single particle radial wave functions are those of a harmonic oscillator. Such matrix elements are encountered in shell-model and Hartree-Fock calculations.

Method of solution
A recursion relation [2] connecting Brody-Moshinsky brackets (B.M.B.) with increasing n_1, n_2 indices is used. The structure of the program is such that a minimum size core is needed to calculate the B.M.B.

Restrictions on the complexity of the problem
In the present form of the program, restrictions come only from the allowed dimensions which are sufficient for values of the indices $n_1, n_2 \leq 5$. For higher values of the indices, these dimensions may easily be increased, so that the size restrictions depend only on the computer storage available.

Typical running time
The running time is 0.40 sec for indices n_1, n_2 equal to 0,1 on the IBM 360/65 computer at the University of Liège.

References
[1] M. Moshinsky, Nucl. Phys. 13 (1959) 104.
[2] T. A. Brody and M. Moshinsky, Tables of transformation brackets (Gordon and Breach, London, 1967).
[3] T. Tamura, Computer Phys. Commun. 1 (1970) 337.

* Chercheur I.I.S.N., on leave from the University of Liège, Belgium.

LONG-WRITE UP

1. INTRODUCTION

The program uses a recursion relation to calculate Brody-Moshinsky Brackets (BMB) for any n_1, n_2 knowing the BMB for $n_1 - 1, n_2$ or $n_1, n_2 - 1$. The procedure is the following. The indices of the BMB generated step by step when the index n_2 decreases are determined; the same is done for the index n_1 at each step of n_2. The BMB for $n_1 = n_2 = 0$ are calculated as well as the intermediate ones needed for the recursion relation which finally leads to the desired BMB. This procedure is carried through with the help of three vectors IC, IA and E. The odd elements of IC indicate the number of BMB generated for each value of n_1 or n_2 given by the next even element of IC. The maximum dimension reached in IC is MC.

The elements of IA are grouped in sets of five elements. Each set describes the indices n', l', N', L' respectively and a number associated with the particular formula for the matrix element $\langle nl, NL, \lambda | -r_1^2 | n'l', N'L', \lambda \rangle$ needed and to be defined below. The maximum dimension reached in IA is MAX. Finally, the vector E collects the intermediate BMB. The second element of E gives the required BMB. The maximum dimension of E is MC/2.

2. MATHEMATICAL METHOD

The formulae coded in this program are described in ref. [1]. The recursion relation used is:

$$\langle nl, NL, \lambda | n_1+1\, l_1, n_2\, l_2, \lambda \rangle = \\ [(n_1+1)(n_1+l_1+\tfrac{3}{2})]^{-1/2} \sum_{n',l',N',L'} \langle nl, NL, \lambda\mu | -r_1^2 | n'l', N'L', \lambda\mu \rangle \langle n'l', N'L', \lambda | n_1 l_1, n_2 l_2, \lambda \rangle , \tag{1}$$

with the energy condition

$$2n + l + 2N + L = 2(n_1+1) + l_1 + 2n_2 + l_2 .$$

This formula enables one to calculate the BMB for n_1+1, n_2 from the BMB for n_1, n_2 and matrix elements of $-r_1^2$. The formulae for these matrix elements may be found in table 1 of ref. [1]. Calculation of any BMB thus implies starting from the BMB for $n_1 = 0$, $n_2 = 0$ [1]:

$$\langle nl, NL, \lambda | 0l_1, 0l_2, \lambda \rangle = \left[\frac{\overline{l_1! l_2!}}{(2l_1)!(2l_2)!} \frac{\overline{(2l+1)(2L+1)}}{2^{l+L}} \frac{\overline{(n+l)!}}{n!(2n+2l+1)!} \frac{(N+L)!}{N!(2N+2L+1)!} \right]^{1/2} \\ \times (-1)^{n+l+L-\lambda} \sum_x (2x+1)\, A(l_1 l, l_2 L, x)\, W(lLl_1 l_2; \lambda x) , \tag{2}$$

the summation index x being limited to the following values:

$$|l - l_1| \leqslant x \leqslant l + l_1 ; \qquad |L - l_2| \leqslant x \leqslant L + l_2 .$$

The function A is defined by:

$$A(l_1 l, l_2 L, x) = \left[\frac{(l_1+l+x+1)!(l_1+l-x)!(l_1+x-l)!}{(l+x-l_1)!} \frac{(l_2+L+x+1)!(l_2+L-x)!(l_2+x-L)!}{(L+x-l_2)!} \right]^{1/2} \\ \times \sum_q (-1)^{\frac{1}{2}(l+q-l_1)} \frac{(l+q-l_1)!}{[\frac{1}{2}(l+q-l_1)]![\frac{1}{2}(l+l_1-q)]!} \frac{1}{(q-x)!(q+x+1)!} \frac{(L+q-l_2)!}{[\frac{1}{2}(L+q-l_2)]![\frac{1}{2}(L+l_2-q)]!} , \tag{3}$$

q being restricted to non negative values for which $l + q - l_1$ is even. Finally, $W(lL_1 l_1 l_2; \lambda x)$ is a Racah coefficient. The program takes care of the energy conservation and of the triangular inequality conditions.

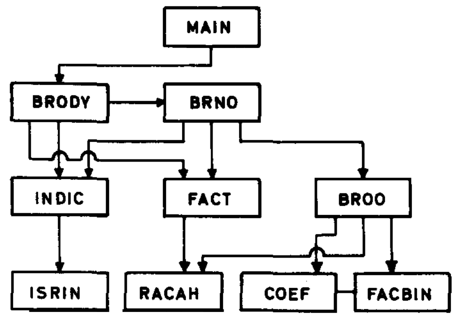
MAIN
BRODY
BRNO
INDIC
FACT
BROO
ISRIN
RACAH
COEF
FACBIN

Fig. 1.

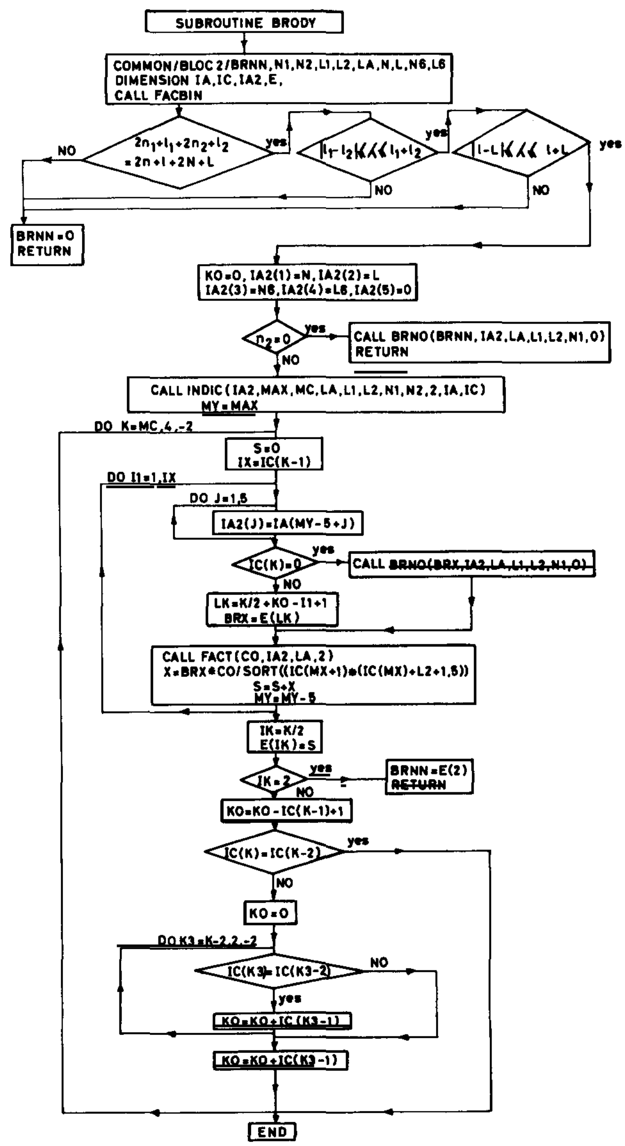
SUBROUTINE BRODY
COMMON/BLOC 2/BRNN,N1,N2,L1,L2,LA,N,L,N6,L6
DIMENSION IA,IC,IA2,E,
CALL FACBIN
2n1+l1+2n2+l2 =2n+l+2N+L
NO
yes
BRNN=0
RETURN
KO=0, IA2(1)=N, IA2(2)=L
IA2(3)=N6, IA2(4)=L6, IA2(5)=0
n2=0
CALL BRNO(BRNN, IA2,LA,L1,L2,N1,0)
RETURN
CALL INDIC(IA2,MAX,MC,LA,L1,L2,N1,N2,2,IA,IC)
MY=MAX
DO K=MC,4,-2
S=0
IX=IC(K-1)
DO I1=1,IX
DO J=1,5
IA2(J)=IA(MY-5+J)
IC(K)=0
CALL BRNO(BRX,IA2,LA,L1,L2,N1,0)
LK=K/2+KO-I1+1
BRX=E(LK)
CALL FACT(CO,IA2,LA,2)
X=BRX*CO/SQRT((IC(MX+1)*(IC(MX)+L2+1.5))
S=S+X
MY=MY-5
IK=K/2
E(IK)=S
IK=2
BRNN=E(2)
RETURN
KO=KO-IC(K-1)+1
IC(K)=IC(K-2)
KO=0
DO K3=K-2,2,-2
IC(K3)=IC(K3-2)
KO=KO+IC(K3-1)
KO=KO+IC(K3-1)
END

Fig. 2.

3. PROGRAM STRUCTURE

The general flow diagram is illustrated by fig. 1.

The main program simply reads the input data N1, N2, L1, L2, LA, N, L, NG, LG which stand for the indices n_1, n_2, l_1, l_2, λ, n, l, N, L respectively of the BMB $\langle nl,NL,\lambda|n_1l_1,n_2l_2,\lambda\rangle$ to be calculated.

Subroutine BRODY calculates the required BMB. Communication between the main program and BRODY is established by the list

COMMON/BLOC2/BRNN, N1, N2, L1, L2, LA, N, L, NG, LG

where BRNN is the desired BMB. The flow diagram for this routine is shown in fig. 2.

Subroutine BRNO (BRNN, IA2, LA, L1, L2, N1, 0) calculates the BMB for $n_2 = 0$; IA2 is a vector of components n, l, N, L.

Subroutine INDIC (IA2, MAX, MC, LA, L1, L2, N1, N2, IH, IA, IC) builds the two vectors IC, IA and calculates their maximum dimensions MC and MAX respectively. The quantity IH is given the value 1 or 2 if INDIC is called by BRODY or BRNO respectively. The flow diagram for INDIC is shown in fig. 3.

Subroutine ISRIN (IA1, IB, K, LA, L1, L2, MH, MK) determines the necessary combinations of n', l', N', L' starting from the input indices IA1 (n, l, N, L); K gives the number of these combinations. The matrix IB contains the resulting indices $n'l'N'L'$ and a number which refers to the special formula to be used for calculating the matrix element of $-r_1^2$. The quantities MH and MK have values associated

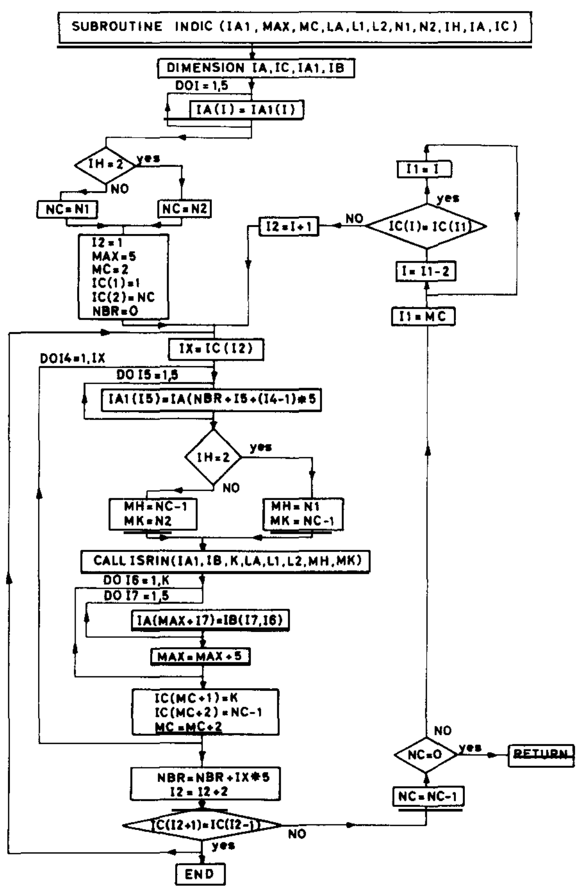

Fig. 3.

with the origin of the CALL ISRIN i.e. either BRODY or BRNO, and serve to ensure the energy conservation rule.

Subroutine FACT (CO, IA2, LA, IH) calculates the matrix elements of $-r_1^2$ or $-r_2^2$. The result is given by CO. Communication with the subroutine RACAH [2] is established by the list

COMMON/BLNJR/RAC, JA, JB, JC, JD, JE, JF

Subroutine BROO (ABRNO, IA2, LA, L1, L2) computes the BMB for $n_1 = n_2 = 0$, the result being the quantity ABRNO. Communication with the subroutines RACAH and FACBIN are established through the list

COMMON/BLOC1/FL(130)/BLNJR/RAC, JA, JB, JC, JD, JE, JF

where the elements of the vector FL are the logarithms of the factorials calculated in FACBIN [2].

Subroutine COEF (L1, L, L2, LG, LX, A) computes the coefficient A given by eq. (3), the index LX corresponding to the index x in eq. (3).

Subroutine FACBIN [2] calculates and stores the logarithms of the factorials required in the calculation. This subroutine is called, once for all, at the beginning of the main subroutine.

Subroutine RACAH has been described in ref. [2].

In its present form, the program provides 200, 1000 and 100 locations for IC, IA and E respectively, which are sufficient for $n_1, n_2 \leq 5$. It is of course possible to increase these locations if necessary.

4. INPUT AND OUTPUT DATA

All the input indices N1, N2, L1, L2, LA, N, L, NG, LG necessary for the calculation of one BMB are integer quantities. These are transmitted to the main subroutine by the first COMMON field. The output data reproduce the above input indices and the corresponding BMB. In the present test run, the calculated BMB can be compared with those contained in ref. [2].

ACKNOWLEDGEMENT

One of us (A. L.) is grateful to Professor Abdus Salam, the International Atomic Energy and UNESCO, for hospitality at the International Centre for Theoretical Physics, Trieste, where an important part of this work has been done.

REFERENCES

[1] T. A. Brody and M. Moshinsky, Tables of transformation brackets (Gordon and Breach, London, 1967).
[2] T. Tamura, Computer Phys. Commun. 1 (1970) 337.

TEST RUN OUTPUT

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COMPUTATION OF THE BRODY-MOSHINSKY COEFFICIENTS

*************************************************************

N1= 0 N2= 0 L1= 5 L2= 6 LA= 6 N= 1 L= 3 NG= 0 LG= 6 BRODY=-0.29514914D 00

N1= 0 N2= 0 L1= 6 L2= 6 LA= 7 N= 1 L= 3 NG= 1 LG= 5 BRODY= 0.18881029D 00

N1= 0 N2= 0 L1= 0 L2= 0 LA= 0 N= 0 L= 0 NG= 0 LG= 0 BRODY= 0.10000000D 01

N1= 0 N2= 0 L1= 6 L2= 6 LA= 0 N= 0 L= 0 NG= 0 LG= 6 BRODY= 0.0

N1= 0 N2= 0 L1= 1 L2= 5 LA= 4 N= 0 L= 5 NG= 0 LG= 1 BRODY=-0.11111111D 00

N1= 0 N2= 0 L1= 3 L2= 4 LA= 5 N= 0 L= 6 NG= 0 LG= 1 BRODY= 0.28490144D-01

N1= 0 N2= 0 L1= 3 L2= 5 LA= 2 N= 0 L= 4 NG= 0 LG= 4 BRODY= 0.0

N1= 0 N2= 0 L1= 5 L2= 5 LA=10 N= 0 L=10 NG= 0 LG= 0 BRODY=-0.49607837D 00

N1= 0 N2= 0 L1= 6 L2= 6 LA=12 N= 0 L=12 NG= 0 LG= 0 BRODY= 0.47495888D 00

N1= 1 N2= 0 L1= 1 L2= 1 LA= 1 N= 0 L= 1 NG= 1 LG= 1 BRODY= 0.50000000D 00

N1= 1 N2= 0 L1= 1 L2= 6 LA= 5 N= 2 L= 4 NG= 0 LG= 1 BRODY=-0.21650635D 00

N1= 1 N2= 0 L1= 2 L2= 6 LA= 5 N= 2 L= 4 NG= 0 LG= 2 BRODY= 0.25000000D 00

N1= 1 N2= 0 L1= 2 L2= 6 LA= 5 N= 0 L= 5 NG= 2 LG= 1 BRODY=-0.22969488D-01

N1= 1 N2= 0 L1= 2 L2= 4 LA= 3 N= 1 L= 4 NG= 0 LG= 2 BRODY=-0.31339159D 00

N1= 1 N2= 0 L1= 2 L2= 4 LA= 5 N= 0 L= 1 NG= 1 LG= 5 BRODY= 0.34069257D 00

N1= 2 N2= 0 L1= 1 L2= 6 LA= 5 N= 0 L= 5 NG= 1 LG= 4 BRODY=-0.10560686D 00

N1= 2 N2= 0 L1= 1 L2= 4 LA= 3 N= 0 L= 0 NG= 3 LG= 3 BRODY= 0.16540766D 00

N1= 2 N2= 0 L1= 2 L2= 4 LA= 5 N= 2 L= 1 NG= 0 LG= 5 BRODY=-0.55901699D-01

N1= 3 N2= 0 L1= 0 L2= 6 LA= 6 N= 1 L= 8 NG= 0 LG= 2 BRODY= 0.19703328D 00

N1= 3 N2= 0 L1= 0 L2= 0 LA= 0 N= 0 L= 0 NG= 3 LG= 0 BRODY= 0.12500000D 00

N1= 3 N2= 0 L1= 0 L2= 3 LA= 3 N= 3 L= 0 NG= 0 LG= 3 BRODY=-0.29041886D-01

N1= 0 N2= 1 L1= 1 L2= 3 LA= 2 N= 0 L= 0 NG= 2 LG= 2 BRODY= 0.19364917D 00

N1= 0 N2= 1 L1= 2 L2= 4 LA= 2 N= 0 L= 3 NG= 1 LG= 3 BRODY=-0.22886885D-01

N1= 0 N2= 1 L1= 4 L2= 4 LA= 8 N= 0 L= 6 NG= 0 LG= 4 BRODY= 0.0

N1= 0 N2= 2 L1= 1 L2= 2 LA= 3 N= 0 L= 0 NG= 2 LG= 3 BRODY= 0.19191237D 00

N1= 0 N2= 2 L1= 2 L2= 2 LA= 4 N= 0 L= 5 NG= 0 LG= 3 BRODY= 0.0

N1= 0 N2= 3 L1= 0 L2= 0 LA= 0 N= 1 L= 1 NG= 1 LG= 1 BRODY=-0.51234754D 00

N1= 1 N2= 1 L1= 1 L2= 1 LA= 2 N= 0 L= 3 NG= 1 LG= 1 BRODY= 0.0

N1= 1 N2= 1 L1= 1 L2= 4 LA= 5 N= 1 L= 1 NG= 1 LG= 4 BRODY=-0.62675374D-01

N1= 1 N2= 1 L1= 4 L2= 4 LA= 8 N= 2 L= 8 NG= 0 LG= 0 BRODY= 0.33572046D 00

N1= 2 N2= 1 L1= 0 L2= 2 LA= 2 N= 0 L= 0 NG= 3 LG= 2 BRODY= 0.27810744D 00

N1= 2 N2= 1 L1= 2 L2= 3 LA= 4 N= 0 L= 1 NG= 3 LG= 4 BRODY= 0.25787450D 00

N1= 1 N2= 2 L1= 1 L2= 1 LA= 2 N= 1 L= 2 NG= 0 LG= 4 BRODY=-0.16431677D 00
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N1= 1 N2= 2 L1= 2 L2= 2 LA= 2 N= 1 L= 4 NG= 0 LG= 4 BRODY=-0.22448980D 00
N1= 2 N2= 2 L1= 0 L2= 0 LA= 0 N= 0 L= 0 NG= 4 LG= 0 BRODY= 0.31374751D 00
N1= 2 N2= 2 L1= 1 L2= 1 LA= 0 N= 1 L= 1 NG= 3 LG= 1 BRODY= 0.0
N1= 2 N2= 1 L1= 1 L2= 3 LA= 2 N= 1 L= 4 NG= 1 LG= 2 BRODY=-0.19254321D 00
N1= 1 N2= 1 L1= 3 L2= 4 LA= 7 N= 1 L= 6 NG= 0 LG= 3 BRODY= 0.39510317D-01
N1= 1 N2= 1 L1= 4 L2= 4 LA= 0 N= 0 L= 0 NG= 6 LG= 0 BRODY= 0.17792089D 00
N1= 2 N2= 2 L1= 2 L2= 2 LA= 0 N= 3 L= 0 NG= 3 LG= 0 BRODY=-0.24756467D 00
N1= 3 N2= 1 L1= 0 L2= 3 LA= 3 N= 0 L= 2 NG= 3 LG= 3 BRODY=-0.19571298D 00
N1= 3 N2= 3 L1= 0 L2= 0 LA= 0 N= 1 L= 4 NG= 1 LG= 4 BRODY= 0.42857143D-01
N1= 3 N2= 3 L1= 0 L2= 0 LA= 0 N= 0 L= 0 NG= 6 LG= 0 BRODY= 0.24464123D 00
N1= 3 N2= 3 L1= 0 L2= 0 LA= 0 N= 6 L= 0 NG= 0 LG= 0 BRODY= 0.24464123D 00
N1= 3 N2= 2 L1= 0 L2= 1 LA= 1 N= 0 L= 5 NG= 0 LG= 6 BRODY= 0.36421568D 00
N1= 3 N2= 2 L1= 0 L2= 2 LA= 2 N= 0 L= 1 NG= 4 LG= 3 BRODY= 0.10940688D 00
N1= 3 N2= 2 L1= 0 L2= 2 LA= 2 N= 3 L= 3 NG= 0 LG= 3 BRODY= 0.41259919D-01
N1= 3 N2= 2 L1= 0 L2= 2 LA= 2 N= 1 L= 4 NG= 1 LG= 4 BRODY= 0.22292421D-01
N1= 3 N2= 2 L1= 0 L2= 2 LA= 2 N= 2 L= 2 NG= 2 LG= 2 BRODY=-0.13505760D 00
N1= 3 N2= 1 L1= 0 L2= 4 LA= 4 N= 1 L= 7 NG= 0 LG= 3 BRODY=-0.20061459D 00
N1= 3 N2= 1 L1= 0 L2= 4 LA= 4 N= 3 L= 2 NG= 1 LG= 2 BRODY= 0.14300057D 00
N1= 3 N2= 1 L1= 0 L2= 3 LA= 3 N= 2 L= 2 NG= 0 LG= 5 BRODY= 0.14923409D 00
N1= 3 N2= 1 L1= 0 L2= 4 LA= 4 N= 1 L= 6 NG= 1 LG= 2 BRODY= 0.12277708D 00
N1= 3 N2= 1 L1= 0 L2= 2 LA= 2 N= 1 L= 2 NG= 2 LG= 2 BRODY=-0.10978876D 00
N1= 3 N2= 1 L1= 0 L2= 3 LA= 3 N= 0 L= 0 NG= 4 LG= 3 BRODY= 0.19974873D 00
N1= 3 N2= 1 L1= 0 L2= 3 LA= 3 N= 0 L= 5 NG= 0 LG= 6 BRODY= 0.22712838D 00
N1= 3 N2= 1 L1= 0 L2= 3 LA= 3 N= 2 L= 1 NG= 2 LG= 2 BRODY=-0.50268050D-01
N1= 3 N2= 1 L1= 0 L2= 2 LA= 2 N= 2 L= 4 NG= 0 LG= 2 BRODY= 0.0
N1= 2 N2= 3 L1= 0 L2= 0 LA= 0 N= 3 L= 1 NG= 1 LG= 1 BRODY= 0.43301270D-01
N1= 2 N2= 2 L1= 2 L2= 2 LA= 4 N= 3 L= 1 NG= 1 LG= 3 BRODY= 0.0
N1= 2 N2= 2 L1= 2 L2= 2 LA= 4 N= 2 L= 6 NG= 0 LG= 2 BRODY=-0.25544431D 00
N1= 2 N2= 2 L1= 2 L2= 2 LA= 2 N= 2 L= 0 NG= 3 LG= 2 BRODY= 0.76459717D-02
N1= 2 N2= 2 L1= 2 L2= 2 LA= 2 N= 3 L= 2 NG= 1 LG= 2 BRODY= 0.23487866D 00
N1= 2 N2= 2 L1= 2 L2= 2 LA= 3 N= 3 L= 3 NG= 1 LG= 1 BRODY=-0.16540766D 00
N1= 3 N2= 3 L1= 0 L2= 0 LA= 0 N= 0 L= 0 NG= 6 LG= 0 BRODY= 0.24464123D 00
N1= 3 N2= 3 L1= 0 L2= 0 LA= 0 N= 4 L= 2 NG= 0 LG= 2 BRODY=-0.30944940D 00
N1= 3 N2= 3 L1= 0 L2= 0 LA= 0 N= 3 L= 2 NG= 1 LG= 2 BRODY=-0.64878222D-01
N1= 3 N2= 3 L1= 0 L2= 0 LA= 0 N= 5 L= 1 NG= 0 LG= 1 BRODY= 0.0
```