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# An efficient algorithm for evaluating the standard Young–Yamanouchi orthogonal representation with two-column Young tableaux for symmetric groups

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**Abstract.** An efficient algorithm for evaluating the standard Young-Yamanouchi orthogonal representation with two-column Young tableaux for symmetric groups is presented. The representation matrix is given as the product of three matrices, where two of them are in triangular form, and are determined by an irreducible representation of the symmetric group, and the other is made up of the elements which equal 1, 0 or −1 according to some simple rules.

## 1. Introduction

The symmetric group approach (SGA) and unitary group approach (UGA) have been widely applied in the study of the many-electron problem in physics and quantum chemistry in the last two decades (Paldus 1974, Hinze 1981, Matsen and Pauncz 1986). It is known that these two methods are deeply interconnected, the representation matrix of a unitary group generator being proportional to the representation matrix of a corresponding cyclic permutation (Wormer and Paldus 1980). Therefore, the symmetric group representation matrices play very important roles in SGA and UGA. The representation theory of the symmetric groups was pioneered by Young and lately by developed by Yamanouchi, Littlewood, Robinson, Hamermesh *et al.* For symmetric groups, there are at least two kinds of irreducible representation. In one the representation matrices are easily obtained, such as the natural representation (Boerner 1963), and the other is orthogonal, such as the so-called Young–Yamanouchi orthogonal representation. Although the former can be directly constructed, because of the non-orthogonality of the representation, it is difficult to apply in physics and quantum chemistry. The latter has been widely used in SGA and UGA, but so far there has not been an efficient method for evaluating the representation matrix of an arbitrary permutation. In the classical treatment, the representation matrix of the transposition $(i, i+1)$ can be directly given, and that of an arbitrary permutation is evaluated from the primitive transpositions of forms $(i, i+1)$ by matrix multiplication. More efficient methods for evaluating the representation matrix of the general transposition $(i, j)$ were given by Rettrup (1977), Paldus and Wormer (1978) and Wilson and Gerratt (1979). Algorithms for calculating the representation matrix of a cyclic permutation have been discussed by Ruttink (1978) and Sahasrabudhe *et al* (1980). All these methods are suitable only for a rather limited class of permutations. Rettrup (1986) presented a compact algorithm by which it is possible to obtain the representation matrix of an arbitrary permutation. But it is also based on matrix multiplication.

In this paper we will present an efficient algorithm for obtaining the standard Young-Yamanouchi orthogonal representation with two-column Young tableaux for symmetric groups by using Young operators. In general, using our algorithm, a representation matrix is expressed as the product of three matrices, where two of them are the triangular intrinsic matrices of the irreducible representation, and determined by the irreducible representation of the symmetric group, and the other can be directly given, its elements taking only three values 1, 0 or −1 according to some simple rules.

In section 2 we shall first discuss the relations between Young operators and the standard projection operators. Although some special relations have been noted (Klein and Junker 1971), we give here the general relations between them, which may be useful in SGA. In section 3, an efficient algorithm for obtaining the standard representation matrices is given by using the transformation matrices between Young operators and the standard projection operators. In sections 4 and 5 some examples and a brief discussion are given respectively. The algorithm presented in this paper can be extended to an arbitrary representation. This problem will be discussed in a later paper.

## 2. Young operators and standard projection operators

It is well known that the matrix elements of the standard representation satisfy the following orthogonality relations:

$$\sum_r D_{rt}^{[\lambda]}(p) D_{ru}^{[\lambda]}(p) = \delta_{tu} \tag{1}$$

$$\sum_u D_{tu}^{[\lambda]}(p) D_{ru}^{[\lambda]}(p) = \delta_{tr} \tag{2}$$

$$\sum_p D_{rs}^{[\lambda]}(p) D_{ut}^{[\lambda']}(p) = \frac{N!}{f_\lambda} \delta_{\lambda\lambda'} \delta_{ru} \delta_{st} \tag{3}$$

$$\sum_{\lambda,r,t} \frac{f_\lambda}{N!} D_{rt}^{[\lambda]}(p) D_{rt}^{[\lambda]}(q) = \delta_{pq} \tag{4}$$

where $D_{rs}^{[\lambda]}(P)$ is the matrix element of the standard Young–Yamanouchi orthogonal representation $[\lambda]$ of the permutation $p$ and $f_\lambda = f$ is the dimension of the irreducible representation $[\lambda]$.

Standard projection operators are defined as

$$e_{rs}^{[\lambda]} = \left(\frac{f_\lambda}{N!}\right)^{1/2} \sum_p D_{rs}^{[\lambda]}(p) p \tag{5}$$

and Young operators are given by

$$E_{rs}^{[\lambda]} = \hat{N}_r \sigma_{rs} \hat{P}_s \tag{6}$$

where $P_r$ and $N_r$ are the row symmetrizer and the column antisymmetrizer of the standard Young tableau $T_r$, respectively, and $\sigma_{rs}$ is the permutation permuting the index numbers of $T_s$ to those of $T_r$. $E_{rs}^{[\lambda]}$ is essentially idempotent and generates a left ideal which yields Young's natural representation (Boerner 1963). Because the decomposition of the representation space into irreducible subspaces is unique, the

Young's natural representation is equivalent to the standard representation. For a given representation $[\lambda]$, we have

$$E_{rs}^{[\lambda]}=\sum_{u,v} a_{uv,rs}e_{uv}^{[\lambda]}. \tag{7}$$

Let us discuss the coefficients $a_{uv,rs}$. Considering

$$E_{f1}^{[\lambda]}=\sum_{u,v} a_{uv,f1}e_{uv}^{[\lambda]}. \tag{8}$$

According to equation (6), for $p_1 \in P_1$, $p_f \in N_f$, we can prove that

$$E_{f1}^{[\lambda]}=\varepsilon_{p_f}p_f E_{f1}^{[\lambda]}p_1=a_{f1,f1}e_{f1}^{[\lambda]} \tag{9}$$

where we used the properties of the representation matrix elements for $[\lambda]=[2^m, 1^l]$,

$$\sum_{p\in P_1} D_{rs}^{[\lambda]}(p)=2^m\delta_{r1}\delta_{s1} \tag{10}$$

$$\sum_{p\in N_1} \varepsilon_p D_{rs}^{[\lambda]}(p)=m!(m+l)!\,\delta_{rf}\delta_{sf} \tag{11}$$

where $P_r$ and $N_r$ are respectively the sets of row and column permutations for the tableau $T_r$, and both are subgroups of $S_N$, $\varepsilon_p=\pm 1$, as $p$ is an even or odd operator. Equation (10) has been proved by Panin (1983), and similarly, equation (11) can be proved.

Comparing the coefficients of elements on both sides of equation (9), we get

$$a_{f1,f1}=\left(\frac{N!}{f_\lambda}\right)^{1/2} D_{f1}^{[\lambda]}(\sigma_{f1}) \tag{12}$$

thus

$$\hat{P}_1\hat{N}_1\hat{P}_1=\frac{1}{m!(m+l)!}a_{f1,f1}^2\left(\frac{N!}{f_\lambda}\right)^{1/2} e_{11}^{[\lambda]}. \tag{13}$$

Comparing the coefficients of the unit element on both sides of equation (13), we have

$$a_{f1,f1}=\pm h_\lambda^{1/2} \tag{14}$$

where $h_\lambda=2^m m!(m+l)!$. It can be proved that $D_{f1}^{[\lambda]}(\sigma_{f1})>0$, thus

$$a_{f1,f1}=h_\lambda^{1/2} \tag{15}$$

$$D_{f1}^{[\lambda]}(a_{f1})=\left(\frac{N!}{f_\lambda h_\lambda}\right)^{1/2} \tag{16}$$

and we have

$$E_{f1}^{[\lambda]}=h_\lambda^{1/2}e_{f1}^{[\lambda]} \tag{17}$$

$$\hat{P}_1\hat{N}_1\hat{P}_1=2^m\left(\frac{N!}{f_\lambda}\right)^{1/2} e_{11}^{[\lambda]} \tag{18}$$

$$\hat{N}_f\hat{P}_f\hat{N}_f=m!(m+l)!\left(\frac{N!}{f_\lambda}\right)^{1/2} e_{ff}^{[\lambda]} \tag{19}$$

where equations (18) and (19) have been presented by Klein and Junker (1971).

From equation (17), it is easy to obtain the relations between Young operators and the standard projection operators.

$$E_{rs}^{[\lambda]} = \sigma_{rf} E_{f1}^{[\lambda]} \sigma_{1s} = h_\lambda^{1/2} \sum_{u,v} D_{fu}^{[\lambda]}(\sigma_{fr}) e_{uv}^{[\lambda]} D_{v1}^{[\lambda]}(\sigma_{s1}). \tag{20}$$

As special cases, we have

$$E_{r1}^{[\lambda]} = h_\lambda^{1/2} \sum_u D_{fu}^{[\lambda]}(\sigma_{fr}) e_{u1}^{[\lambda]} \tag{21}$$

$$E_{fr}^{[\lambda]} = h_\lambda^{1/2} \sum_u D_{u1}^{[\lambda]}(\sigma_{r1}) e_{fu}^{[\lambda]}. \tag{22}$$

If we define the square matrices $E$, $e$, $A$ and $B$ as follows:

$$(E)_{rs} = E_{rs}^{[\lambda]} \tag{23}$$

$$(e)_{rs} = e_{rs}^{[\lambda]} \tag{24}$$

$$(A)_{rs} = D_{fr}^{[\lambda]}(\sigma_{fs}) \tag{25}$$

$$(B)_{rs} = D_{r1}^{[\lambda]}(\sigma_{s1}) \tag{26}$$

and define the row matrices $E_1$, $E_f$, $e_1$ and $e_f$ as

$$E_1 = (E_{11}^{[\lambda]}, E_{21}^{[\lambda]}, \ldots, E_{f1}^{[\lambda]}) \tag{27}$$

$$E_f = (E_{f1}^{[\lambda]}, E_{f2}^{[\lambda]}, \ldots, E_{ff}^{[\lambda]}) \tag{28}$$

$$e_1 = (e_{11}^{[\lambda]}, e_{21}^{[\lambda]}, \ldots, e_{f1}^{[\lambda]}) \tag{29}$$

$$e_f = (e_{f1}^{[\lambda]}, e_{f2}^{[\lambda]}, \ldots, e_{ff}^{[\lambda]}). \tag{30}$$

Equations (20)-(22) can be rewritten as

$$E = h_\lambda^{1/2} \tilde{A} e B \tag{31}$$

$$E_1 = h_\lambda^{1/2} e_1 A \tag{32}$$

$$E_f = h_\lambda^{1/2} e_f B. \tag{33}$$

Equations (21) and (22) imply that the relations between $E_{r1}^{[\lambda]}$ and $e_{s1}^{[\lambda]}$ and between $E_{fr}^{[\lambda]}$ and $e_{fs}^{[\lambda]}$ are linear. It can be found that the transformation matrices $A$ and $B$ are in triangular form. Generally, the direct product of both matrices is the transformation matrix between $E_{rs}^{[\lambda]}$ and $e_{ut}^{[\lambda]}$.

Comparing the coefficients of the same permutation on both sides of equation (17), we have

$$D_{f1}^{[\lambda]}(\pi) = \begin{cases} \varepsilon_{\pi_1}(N!/f_\lambda h_\lambda)^{1/2} & \text{if } \pi = \pi_1 \sigma_{f1} \pi_2 \qquad \pi_1 \in N_f \qquad \pi_2 \in P_1 \\ 0 & \text{otherwise.} \end{cases} \tag{34}$$

## 3. The algorithm for evaluating the matrix elements of the standard Young–Yamanouchi orthogonal representation

For any given permutation $\pi$, we have

$$D_{uv}^{[\lambda]}(\sigma_{ur}\pi\sigma_{sv}) = \sum_{k,l} D_{uk}^{[\lambda]}(\sigma_{ur}) D_{kl}^{[\lambda]}(\pi) D_{lv}^{[\lambda]}(\sigma_{sv}) \qquad u, v = 1, 2, \ldots, f \tag{35}$$

For any given indices $u$, $v$, defining the matrices $D(\pi)$, $U$, $V$ and $W(\pi)$ as follows:

$$[D(\pi)]_{rs}=D^{[\lambda]}_{rs}(\pi) \tag{36}$$

$$(U)_{rs}=D^{[\lambda]}_{ur}(\sigma_{us}) \tag{37}$$

$$(V)_{rs}=D^{[\lambda]}_{rv}(\sigma_{sv}) \tag{38}$$

$$[W(\pi)]_{rs}=D^{[\lambda]}_{uv}(\sigma_{ur}\pi\sigma_{sv}) \tag{39}$$

we have

$$D(\pi)=\tilde{U}^{-1}W(\pi)V^{-1}. \tag{40}$$

From equation (40), it may be obtained that:
(i) if $u, v=f$, then

$$W(\pi)=(W(\pi)_{rs})=D^{[\lambda]}_{ff}(\sigma_{fr}\pi\sigma_{sf}) \tag{41}$$

$$D(\pi)=\tilde{A}^{-1}W(\pi)A^{-1}. \tag{42}$$

(ii) if $u, v=1$, then

$$W(\pi)=(W(\pi)_{rs})=D^{[\lambda]}_{11}(\sigma_{1r}\pi\sigma_{s1}) \tag{43}$$

$$D(\pi)=\tilde{B}^{-1}W(\pi)B^{-1}. \tag{44}$$

(iii) if $u=f$, $v=1$, then

$$W(\pi)=(W(\pi)_{rs})=D^{[\lambda]}_{f1}(\sigma_{fr}\pi\sigma_{s1}) \tag{45}$$

$$D(\pi)=\tilde{A}^{-1}W(\pi)B^{-1}. \tag{46}$$

Because it is easy to obtain the elements $D^{[\lambda]}_{11}(\pi)$, $D^{[\lambda]}_{ff}(\pi)$ and $D^{[\lambda]}_{f1}(\pi)$ (Goddard 1967, Zhang and Li 1989), equations (42), (44) and (46) provide algorithms for evaluating the standard Young-Yamanouchi representation matrices, where the representation matrix $D(\pi)$ can be expressed as the product of three matrices. Here we focus our attention on the third algorithm, equation (46). Defining

$$E^{[\lambda]}_{rs}=\sum_{\pi} C_{rs}(\pi)\pi \tag{47}$$

and using

$$E^{[\lambda]}_{rs}=\sigma_{ru}E^{[\lambda]}_{uv}\sigma_{vs}=\sum_{\pi} C_{uv}(\pi)\sigma_{ru}\pi\sigma_{vs}=\sum_{\pi} C_{uv}(\sigma_{ur}\pi\sigma_{sv})\pi \tag{48}$$

for any given indices $r$, $s$, $u$, $v$, we have

$$C_{rs}(\pi)=C_{uv}(\sigma_{ur}\pi\sigma_{sv}). \tag{49}$$

For example,

$$C_{rs}(\pi)=C_{11}(\sigma_{1r}\pi\sigma_{s1})=C_{ff}(\sigma_{fr}\pi\sigma_{sf})=C_{f1}(\sigma_{fr}\pi\sigma_{s1}). \tag{50}$$

From equations (17) and (50), we have

$$D^{[\lambda]}_{f1}(\sigma_{fr}\pi\sigma_{s1})=\left(\frac{N!}{f_\lambda h_\lambda}\right)^{1/2}C_{f1}(\sigma_{fr}\pi\sigma_{s1})=\left(\frac{N!}{f_\lambda h_\lambda}\right)^{1/2}C_{rs}(\pi). \tag{51}$$

Equation (46) may be rewritten as

$$D(\pi)=\left(\frac{N!}{f_\lambda h_\lambda}\right)^{1/2}\tilde{A}^{-1}C(\pi)B^{-1}. \tag{52}$$

It is evident from equation (50) that the element $[C(\pi)]_{rs}$ may be obtained by the following steps:

(i) writing the corresponding permutation $\pi' = \delta_{1r}\pi\sigma_{s1}$;

(ii) dividing the index numbers of $\pi'$ into several sets according to whether they are in the first or the second column of $T_1$, for example,

$$\pi' = (\alpha_{i_1} \ldots \alpha_{i_2}, \beta_{i_3} \ldots \beta_{i_4}, \alpha_{i_3} \ldots)(\ldots)$$

where $\alpha_i$ and $\beta_i$ are the index numbers in the first and the second columns of $T_1$, respectively;

(iii) retaining the last index number in every set, and deleting other index numbers, or deleting an independent cycle if there is only one set in it;

(iv) if the number of index numbers retained is even, and for any given $\beta_i$, there is a corresponding index number $\alpha_i = \beta_i - 1$, $[C(\pi)]_{rs} = (-1)^{\mu+\nu}$, otherwise $[C(\pi)]_{rs} = 0$, where $\mu$ and $\nu$ are the numbers of indices and cycles deleted, respectively.

Using

$$D_{ff}^{[\lambda]}(\sigma_{fr}\sigma_{sf}) = \sum_u D_{fu}^{[\lambda]}(\sigma_{fr}) D_{uf}^{[\lambda]}(\sigma_{sf})$$

$$\sum_r [D_{fr}^{[\lambda]}(\sigma_{fs})]^2 - 1 \qquad s = 1, 2, \ldots, f$$

we have the following recursion formula:

$$A_{rs} = \begin{cases} \left[ D_{ff}^{[\lambda]}(\sigma_{fr}\sigma_{sf}) - \sum\limits_{u>r} A_{ur}A_{us} \right] \Big/ A_{rr} & r > s \\ \left( 1 - \sum\limits_{u>r} A_{ur}^2 \right)^{1/2} & r = s \\ 0 & r < s. \end{cases} \tag{53}$$

From equation (53), we can obtain $A$ in order as $A_{ff}, A_{f-1f}, \ldots, A_{1f}; A_{ff-1}, \ldots, A_{11}$. Similarly, we can obtain $B$ by

$$B_{rs} = \begin{cases} \left[ D_{11}^{[\lambda]}(\sigma_{1r}\sigma_{s1}) - \sum\limits_{u<r} B_{ur}B_{us} \right] \Big/ B_{rr} & r < s \\ \left( 1 - \sum\limits_{u<r} B_{ur}^2 \right)^{1/2} & r = s \\ 0 & r > s. \end{cases} \tag{54}$$

## 4. Examples

For $N = 4, S = l/2 = 1$,

$$\begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & \\ \cline{1-1} 4 & \\ \cline{1-1} \end{array} \qquad \begin{array}{|c|c|} \hline 1 & 3 \\ \hline 2 & \\ \cline{1-1} 4 & \\ \cline{1-1} \end{array} \qquad \begin{array}{|c|c|} \hline 1 & 4 \\ \hline 2 & \\ \cline{1-1} 3 & \\ \cline{1-1} \end{array}$$

| $r$ | 1 | 2 | 3 |
|---|---|---|---|
| $\sigma_{r1}$ | $e$ | (23) | (243) |
| $\sigma_{rf}$ | (234) | (34) | $e$ |

For $[\lambda]=[2,1^2]$, the intrinsic matrices $A$ and $B$ are given by

$$A=\begin{pmatrix} \frac{\sqrt{6}}{3} & 0 & 0 \\ \frac{\sqrt{2}}{3} & \frac{2\sqrt{2}}{3} & 0 \\ -\frac{1}{3} & \frac{1}{3} & 1 \end{pmatrix} \qquad B=\begin{pmatrix} 1 & -\frac{1}{2} & \frac{1}{2} \\ 0 & \frac{\sqrt{3}}{2} & -\frac{\sqrt{3}}{6} \\ 0 & 0 & \frac{\sqrt{6}}{3} \end{pmatrix}$$

for $\pi=(14)$,

$$\pi'=\begin{pmatrix} (14) & (14)(23) & (1432) \\ (14)(23) & (14) & (142) \\ (1234) & (124) & (12) \end{pmatrix}$$

$$C[(14)]=\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 1 & -1 & 1 \end{pmatrix}$$

$$D[(14)]=\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{6} & \frac{\sqrt{6}}{3} \\ -\frac{\sqrt{3}}{6} & -\frac{5}{6} & -\frac{\sqrt{2}}{3} \\ \frac{\sqrt{6}}{3} & -\frac{\sqrt{2}}{3} & \frac{1}{3} \end{pmatrix}.$$

Similarly,

$$C[(124)]=\begin{pmatrix} -1 & 1 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

thus

$$D[(124)]=\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{6} & -\frac{\sqrt{6}}{3} \\ -\frac{\sqrt{3}}{5} & \frac{5}{6} & \frac{\sqrt{2}}{3} \\ \frac{\sqrt{6}}{3} & \frac{\sqrt{2}}{3} & -\frac{1}{3} \end{pmatrix}.$$

## 5. Discussion

In this paper we have given a direct method for evaluating the standard Young–Yamanouchi orthogonal representation matrices which is more efficient than those used up to the present. For instance, for $\pi=(18)$, multiplication of 13 matrices corresponding to transpositions is involved in the traditional treatment, but we only need three matrices, where two triangular matrices are determined by an irreducible representation of the symmetric groups.

It is worthy of note that for some irreducible representations, we have

$$\tilde{B}=\left(\frac{N!}{f_\lambda h_\lambda}\right)^{1/2} A^{-1}. \tag{55}$$

For instance, for $N=3$, $S=\frac{1}{2}$; $N=4$, $S=0$; $N=5$, $S=\frac{3}{2}$; $N=6$, $S=2$, $A$ and $B$ satisfy equation (55). It implies that $C(\pi)$ is an irreducible representation of the symmetric group. For arbitrary irreducible representations, we have

$$D'(\pi)=B^{-1}D(\pi)B=\left(\frac{N!}{f_\lambda h_\lambda}\right)^{1/2}(\tilde{A}B)^{-1}C(\pi). \tag{56}$$

It is clear that $D'(\pi)$ is also an irreducible representation and similar to that presented by Gallup (1972).

In this paper we have presented the transformation relations between the standard projection operators and Young operators which could connect the group algebra method with the representation theory of symmetric groups. Using these formulae on one hand, the representation matrices of symmetric groups are obtained by Young operators, and on the other hand, some properties of Young operators may easily be derived by using the representation theory. For instance, it is evident from equation (20) that

$$E_{rs}^{[\lambda]}E_{tu}^{[\lambda']}=\delta_{\lambda\lambda'}\frac{N!}{f_\lambda}C_{ts}(I)E_{ru}^{[\lambda]}. \tag{57}$$

Equation (57) was presented by Rutherford (1948) who used complicated group algebra operations.

We have discussed the irreducible representation matrices only for the two-column Young tableau in this paper. There is a similar algorithm for an arbitrary representation, which will be discussed in a later paper.

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## Appendix. Matrices $\tilde{A}^{-1}$ and $B^{-1}$

$N=3$, $S=\frac{1}{2}$; $N=4$, $S=0$:

$$\tilde{A}^{-1}=\begin{pmatrix}\frac{2\sqrt{3}}{3} & -\frac{\sqrt{3}}{3}\\ 0 & 1\end{pmatrix}\qquad B^{-1}=\begin{pmatrix}1 & \frac{\sqrt{3}}{3}\\ 0 & \frac{2\sqrt{3}}{3}\end{pmatrix}$$

$N=4$, $S=1$:

$$\tilde{A}^{-1}=\begin{pmatrix}\frac{\sqrt{6}}{2} & -\frac{\sqrt{6}}{4} & \frac{\sqrt{6}}{4}\\ 0 & \frac{3\sqrt{2}}{4} & -\frac{\sqrt{2}}{4}\\ 0 & 0 & 1\end{pmatrix}\qquad B^{-1}=\begin{pmatrix}1 & \frac{\sqrt{3}}{3} & -\frac{\sqrt{6}}{6}\\ 0 & \frac{2\sqrt{3}}{3} & \frac{\sqrt{6}}{6}\\ 0 & 0 & \frac{\sqrt{6}}{2}\end{pmatrix}$$

$N=5$, $S=\frac{3}{2}$:

$$\tilde{A}^{-1}=\begin{pmatrix} \frac{2\sqrt{10}}{5} & -\frac{\sqrt{10}}{5} & \frac{\sqrt{10}}{5} & -\frac{\sqrt{10}}{5} \\ 0 & \frac{\sqrt{30}}{5} & -\frac{\sqrt{30}}{15} & \frac{\sqrt{30}}{15} \\ 0 & 0 & \frac{4\sqrt{15}}{15} & -\frac{\sqrt{15}}{15} \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$B^{-1}=\begin{pmatrix} 1 & \frac{\sqrt{3}}{3} & -\frac{\sqrt{6}}{6} & \frac{\sqrt{10}}{10} \\ 0 & \frac{2\sqrt{3}}{3} & \frac{\sqrt{6}}{6} & -\frac{\sqrt{10}}{10} \\ 0 & 0 & \frac{\sqrt{6}}{2} & \frac{\sqrt{10}}{10} \\ 0 & 0 & 0 & \frac{2\sqrt{10}}{10} \end{pmatrix}$$

$N=5$, $S=\frac{1}{2}$; $N=6$, $S=0$:

$$\tilde{A}^{-1}=\begin{pmatrix} \sqrt{2} & -\frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{4} & -\frac{3\sqrt{2}}{4} \\ 0 & \frac{\sqrt{6}}{2} & 0 & -\frac{\sqrt{6}}{4} & \frac{\sqrt{6}}{4} \\ 0 & 0 & \frac{\sqrt{6}}{2} & -\frac{\sqrt{6}}{4} & \frac{\sqrt{6}}{4} \\ 0 & 0 & 0 & \frac{3\sqrt{2}}{4} & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$B^{-1}=\begin{pmatrix} 1 & \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} & \frac{1}{3} & -\frac{\sqrt{2}}{6} \\ 0 & \frac{2\sqrt{3}}{3} & 0 & \frac{2}{3} & -\frac{\sqrt{2}}{3} \\ 0 & 0 & \frac{2\sqrt{3}}{3} & \frac{2}{3} & -\frac{\sqrt{2}}{3} \\ 0 & 0 & 0 & \frac{4}{3} & \frac{\sqrt{2}}{3} \\ 0 & 0 & 0 & 0 & \sqrt{2} \end{pmatrix}$$

$N=6$, $S=2$:

$$\tilde{A}^{-1}=\begin{pmatrix} \frac{\sqrt{15}}{3} & -\frac{\sqrt{15}}{6} & \frac{\sqrt{15}}{6} & -\frac{\sqrt{15}}{6} & \frac{\sqrt{15}}{6} \\ 0 & \frac{\sqrt{5}}{2} & -\frac{\sqrt{5}}{6} & \frac{\sqrt{5}}{6} & -\frac{\sqrt{5}}{6} \\ 0 & 0 & \frac{\sqrt{10}}{3} & -\frac{\sqrt{10}}{12} & \frac{\sqrt{10}}{12} \\ 0 & 0 & 0 & \frac{5\sqrt{6}}{12} & -\frac{\sqrt{6}}{12} \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$B^{-1}=\begin{pmatrix} 1 & \frac{\sqrt{3}}{3} & -\frac{\sqrt{6}}{6} & \frac{\sqrt{10}}{10} & -\frac{\sqrt{15}}{15} \\ 0 & \frac{2\sqrt{3}}{3} & \frac{\sqrt{6}}{6} & -\frac{\sqrt{10}}{10} & \frac{\sqrt{15}}{15} \\ 0 & 0 & \frac{\sqrt{6}}{2} & \frac{\sqrt{10}}{10} & -\frac{\sqrt{15}}{15} \\ 0 & 0 & 0 & \frac{2\sqrt{10}}{5} & \frac{\sqrt{15}}{15} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{15}}{3} \end{pmatrix}$$

$N=6$, $S=1$:

$$\tilde{A}^{-1}=\begin{pmatrix} \frac{2\sqrt{15}}{5} & -\frac{\sqrt{15}}{5} & \frac{\sqrt{15}}{5} & -\frac{\sqrt{15}}{5} & \frac{\sqrt{15}}{10} & -\frac{\sqrt{15}}{10} & -\frac{3\sqrt{15}}{10} & \frac{\sqrt{15}}{6} & -\frac{\sqrt{15}}{6} \\ 0 & \frac{3\sqrt{5}}{6} & -\frac{\sqrt{5}}{5} & 0 & -\frac{3\sqrt{5}}{10} & \frac{\sqrt{5}}{10} & \frac{3\sqrt{5}}{10} & \frac{\sqrt{5}}{30} & \frac{11\sqrt{5}}{30} \\ 0 & 0 & \frac{2\sqrt{10}}{5} & 0 & 0 & -\frac{\sqrt{10}}{5} & 0 & -\frac{\sqrt{10}}{15} & -\frac{2\sqrt{10}}{15} \\ 0 & 0 & 0 & \frac{3\sqrt{5}}{5} & -\frac{3\sqrt{5}}{10} & \frac{3\sqrt{5}}{10} & \frac{3\sqrt{5}}{10} & -\frac{3\sqrt{5}}{10} & \frac{\sqrt{5}}{5} \\ 0 & 0 & 0 & 0 & \frac{3\sqrt{15}}{10} & -\frac{\sqrt{15}}{10} & -\frac{\sqrt{15}}{10} & \frac{\sqrt{15}}{30} & -\frac{2\sqrt{15}}{15} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{5} & 0 & -\frac{\sqrt{30}}{15} & \frac{\sqrt{30}}{15} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{5} & -\frac{\sqrt{30}}{15} & \frac{\sqrt{30}}{15} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{4\sqrt{15}}{15} & \frac{\sqrt{15}}{15} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & \frac{\sqrt{3}}{6} & -\frac{\sqrt{6}}{6} & \frac{\sqrt{3}}{3} & \frac{1}{3} & -\frac{\sqrt{2}}{6} & -\frac{2\sqrt{2}}{3} & \frac{2}{3} & 0 \end{pmatrix}$$

$$B^{-1}=\begin{pmatrix} 1 & \frac{\sqrt{3}}{6} & -\frac{\sqrt{6}}{6} & \frac{\sqrt{3}}{3} & \frac{1}{3} & -\frac{\sqrt{2}}{6} & -\frac{2\sqrt{2}}{3} & \frac{2}{3} & 0 \\ 0 & \frac{2\sqrt{3}}{3} & \frac{\sqrt{6}}{6} & 0 & \frac{2}{3} & \frac{\sqrt{2}}{6} & -\frac{\sqrt{2}}{3} & -\frac{1}{6} & \frac{\sqrt{15}}{30} \\ 0 & 0 & \frac{\sqrt{6}}{2} & 0 & 0 & \frac{\sqrt{2}}{2} & 0 & -\frac{1}{2} & \frac{\sqrt{15}}{10} \\ 0 & 0 & 0 & \frac{2\sqrt{3}}{3} & \frac{2}{3} & -\frac{\sqrt{2}}{3} & -\frac{\sqrt{2}}{3} & \frac{1}{3} & \frac{\sqrt{15}}{15} \\ 0 & 0 & 0 & 0 & \frac{4}{3} & \frac{\sqrt{2}}{3} & \frac{\sqrt{2}}{3} & \frac{1}{6} & \frac{\sqrt{15}}{10} \\ 0 & 0 & 0 & 0 & 0 & \sqrt{2} & 0 & \frac{1}{2} & -\frac{\sqrt{10}}{15} \\ 0 & 0 & 0 & 0 & 0 & 0 & \sqrt{2} & \frac{1}{2} & -\frac{\sqrt{15}}{10} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{3}{2} & \frac{\sqrt{15}}{10} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{2\sqrt{15}}{5} \end{pmatrix}$$

## References


Boerner H 1963 *Representations of Groups* (New York: Wiley)
Gallup G A 1972 *Int. J. Quantum Chem.* **6** 761
Goddard W A 1967 *Phys. Rev.* **157** 73
Hinze J 1981 *The Unitary Group for the Evaluation of Electronic Energy Matrix Elements (Lecture Notes in Chemistry 22)* (Berlin: Springer)
Klein D J and Junker B R 1971 *J. Chem. Phys.* **54** 4290
Matsen F A and Pauncz R 1986 *The Unitary Group in Quantum Chemistry* (Amsterdam: Elsevier)
Paldus J 1974 *J. Chem. Phys.* **61** 5321
Paldus J and Wormer P E S 1978 *Phys. Rev.* A **18** 827
Panin A I 1983 *Int. J. Quantum Chem.* **24** 279
Rettrup S 1977 *Chem. Phys. Lett.* **47** 59
—— 1986 *Int. J. Quantum Chem.* **29** 119
Rutherford D E 1948 *Substitutional Analysis* (Edinburgh: Edinburgh University Press)
Ruttink P J A 1978 *Theor. Chem. Acta* **49** 223
Sahasrabudhe G G, Dinesha K V and Sarma C R 1980 *Theor. Chim. Acta* **54** 333
Wilson S and Gerratt J 1979 *J. Phys. B: At. Mol. Phys.* **18** 339
Wormer P E S and Paldus J 1980 *Int. J. Quantum Chem.* **18** 41
Zhang Q and Li X 1989 *J. Mol. Structure* **198** 413