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MATRIX ELEMENTS OF THE SPIN-SPIN
INTERACTIONS FOR f^4 CONFIGURATIONS*

J. A. Barnes, B. L. Carroll and L. M. Flores
Lockheed Electronics Company, Houston, Texas

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ABSTRACT

The Spin-Spin matrix elements for f^4 electron configurations are computed and tabulated for general usage.

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Introduction:

The introduction of mutual magnetic interactions arising from relativistic corrections to the many-electron atom should lead to improvement in theoretical multiplet structure calculations.

Previously, researchers have made available tables of the Spin-Spin¹ and Spin-Other-Orbit² interactions for f^3 configurations. Judd, et al^{3,4} have presented the Spin-Spin and Spin-Other-Orbit matrix elements for diagonal terms of maximum multiplicity in f^n systems. In this paper we present the Spin-Spin matrix elements for f^4 configurations.

Matrix Elements of the Spin-Spin Interaction:

The matrix elements of the Spin-Spin interaction for f^n configurations⁵ can be written in tensor operator form as,

$$\langle f^n \gamma S L J | H_{SS} | f^n \gamma' S' L' J' \rangle = \delta(J, J') (-1)^{S'+L+J} \begin{Bmatrix} S & S' & 2 \\ L' & L & J \end{Bmatrix} \\ \times \langle f^n \gamma S L | | H_{SS} | | f^n \gamma' S' L' \rangle . \quad (1)$$

The reduced matrix elements of H_{ss} , occurring in Eq. (1) are given by

$$(f^n \gamma SL || H_{ss} || f^{n'} \gamma' S' L') = \sum_k z_k M^{k-1} \sum_{\gamma \bar{S} \bar{L}} (f^n \gamma SL || V^{(1,k-1)} || f^{n'} \gamma' \bar{S} \bar{L}) \\ \times (f^{n'} \gamma' \bar{S} \bar{L} || V^{(1,k+1)} || f^n \gamma S L) (-1)^{S+L+S'+L'} \\ \times \begin{Bmatrix} S & S' & 2 \\ 1 & 1 & S'' \end{Bmatrix} \begin{Bmatrix} L' & L & 2 \\ k-1 & k+1 & L''' \end{Bmatrix} \quad (2)$$

where

$$z_k = -4 \{ 5k(k+1)(2k-1)(2k+1)(2k+3) \}^{1/2} \\ \times (3 || C^{(k-1)} || 3) (3 || C^{(k+1)} || 3) . \quad (3)$$

The reduced matrix elements of the double tensor operator $V^{(1,k)}$, and the tensor operator C^k , are defined by,

$$(f^n \gamma SL || V^{(1,k)} || f^{n'} \gamma' S' L') = n \{ (3/2)(2S+1)(2L+1)(2S'+1)(2L'+1) \}^{1/2} \\ \times \sum_{\gamma \bar{S} \bar{L}} (f^n \gamma SL \{ | f^{n-1} \gamma \bar{S} \bar{L} \} (f^{n-1} \gamma \bar{S} \bar{L} |) f^{n'} \gamma' S' L') \\ \times \begin{Bmatrix} S & S' & 1 \\ 1/2 & 1/2 & \bar{S} \end{Bmatrix} \begin{Bmatrix} L & L' & K \\ 3 & 3 & \bar{L} \end{Bmatrix} \\ \times (-1)^{\bar{S}+\bar{L}+S+L+1/2+K} , \quad (4)$$

and

$$(3||C^k||3) = -7 \begin{pmatrix} 3 & k & 3 \\ 0 & 0 & 0 \end{pmatrix} . \quad (5)$$

In Eqs. (1) thru (5) ,

$$\begin{pmatrix} a & b & c \\ 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad \begin{Bmatrix} a & b & c \\ d & e & f \end{Bmatrix}$$

are the Wigner 3-j and 6-j symbols. The coefficients ($f^n \gamma_{SL} | f^{n-1} \bar{\gamma}_{SL} \rangle$) are the coefficients of fractional parentage introduced by Racah⁶ and tabulated by Nielson and Koster⁷. The radial integral, $M^{(k-1)}$, is defined by Marvin⁸ as ,

$$M^{(k-1)} = \left(\frac{1}{4c^2} \right) \int_{r_j > r_i} \int P^2 n_1(r_i) \left(\frac{r_i^{k-1}}{r_j^{k+2}} \right) P_{n_1}(r_j) dr_i dr_j ,$$

where P_{n_1} is the radial wave function for the shell (n_1) and c is the speed of light.

Discussion of Table:

Table I presents a tabulation of the matrix elements of the Spin-Spin operator H_{ss} for f^4 configurations. The calculations were performed in single precision on the Univac 1108 computer. A comparison with the diagonal matrix elements of maximum multiplicity for f^4 presented by Judd³ indicates an accuracy of at least seven significant figures.

The matrix elements are tabulated in J-blocks. The states $| (U\tau v)SL \rangle$ labeling a given J-block are listed in parenthesis beside the J-value⁹. The matrices of H_{SS} are presented in upper-half diagonal form. Only the non-zero elements are listed for a given J-block. Each matrix element is given as the sum of three terms, one for each radial integral M^k . In a given J-block, the coefficients of the M^k 's are listed in rows to the right of the desired matrix element. Each entry in the table is to be multiplied by the power of ten indicated by its following single digit.

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⁹The state notation may be related to that used by Nielson and Koster⁷ through the use of their tables presented on pages 2 and 3.

TABLE I. SPIN-SPIN INTERACTION OF f^4 ELECTRONS FOR VARIOUS J LEVELS.^a

$J = 10.0$	$(3004)3M$	$(2204)1N$	M^0	M^2	M^4	$(U_{TV})SL$	$(U' \tau' v')S'L'$	M^0	M^2	M^4	$(U_{TV})SL$	$(U' \tau' v')S'L'$	M^0	M^2	M^4
$(3004)3M$	$(3004)3M$	$-3.999998-1$	$1.478787+0$	$-2.362788+0$											
$J = 9.0$	$(2104)3L$	$(3004)3M$	M^0	M^2	M^4	$(U_{TV})SL$	$(U' \tau' v')S'L'$	M^0	M^2	M^4	$(U_{TV})SL$	$(U' \tau' v')S'L'$	M^0	M^2	M^4
$(2104)3L$	$(2104)3L$	0.000000	$-8.888883-1$	$1.977819+0$	$(3004)3M$	$(3004)3M$	$9.333328-1$	$-3.450503+0$	$5.513171+0$						
$J = 8.0$	$(2004)5I$	$(2104)3K$	$(3004)3K$	$(2104)3L$	$(3004)3M$	$(2104)3L$	$(3004)3M$	$(2104)1L$	$(2204)1L$						
$(U_{TV})SL$	$(U' \tau' v')S'L'$	M^0	M^2	M^4	$(U_{TV})SL$	$(U' \tau' v')S'L'$	M^0	M^2	M^4	$(U_{TV})SL$	$(U' \tau' v')S'L'$	M^0	M^2	M^4	
$(2004)5I$	$(2004)5I$	$-7.999996-1$	$-3.393938-1$	$-1.936850+0$	$(2104)3L$	$-5.163975-1$	$4.514566+0$	$-4.256805+0$							
$(2104)3K$	$2.309400-1$	$9.132627-1$	$-4.690738+0$	$(3004)3M$	$-1.091859+0$	$1.455812+0$	$1.992717+0$								
$(3004)3K$	$-1.904380+0$	$4.587824+0$	$1.921934+0$	$(3004)3K$	$-2.954247-1$	$-5.670822-1$	$-8.121937-1$								
$(2104)3L$	$2.683280+0$	$-2.561313+0$	$-2.558754+0$	$(2104)3L$	$1.252448+0$	$-1.909034+0$	$-3.309936+0$								
$(2104)1L$	0.000000	$-8.049430-1$	$-8.443455-1$	$(3004)3M$	$-2.118517+0$	$5.617283-2$	$3.012063+0$								
$(2204)1L$	0.000000	$-2.241604+0$	$5.486442-1$	$(2104)3L$	0.000000	$2.111110+0$	$-4.697320+0$								
$(2104)3K$	$-8.988886-2$	$-8.343429-1$	$3.715474-1$	$(3004)3M$	$-1.409583+0$	$2.221162+0$	$4.036236+0$								
$(3004)3K$	$-4.958553-1$	$-3.106414-1$	$1.268527+0$	$(3004)3M$	$(3004)3M$	$-5.490193-1$	$2.029708+0$	$-3.243042+0$							
$J = 7.0$	$(2004)5I$	$(2004)3I$	$(2004)3I$	$(2104)3K$	$(3004)3K$	$(2104)3K$	$(3004)3K$	$(2104)1K$							
$(U_{TV})SL$	$(U' \tau' v')S'L'$	M^0	M^2	M^4	$(U_{TV})SL$	$(U' \tau' v')S'L'$	M^0	M^2	M^4	$(U_{TV})SL$	$(U' \tau' v')S'L'$	M^0	M^2	M^4	
$(2004)5I$	$(2004)5I$	$7.999996-1$	$3.393938-1$	$1.936850+0$	$(2104)3L$	$-7.197879-1$	$1.864905+0$	$-3.878069+0$							
$(2004)3I$	$1.920316+0$	$-2.348816+0$	$-3.792799+0$	$(3004)3I$	$(3004)3I$	$3.809521-2$	$1.281384+0$	$4.171583-1$							
$(3004)3I$	$-1.842288+0$	$1.227811+0$	$1.438490+0$	$(2104)3K$	$4.952377-1$	$-6.360747-1$	$-3.832428+0$								
$(2104)3K$	$-2.519761-1$	$-9.964513-1$	$5.118015+0$	$(3004)3K$	$6.282823-1$	$-1.822571+0$	$-2.554601-1$								
$(3004)3K$	$2.077849+0$	$-5.005726+0$	$-2.097002+0$	$(2104)3L$	$-1.246709+0$	$5.100174+0$	$-1.931884+0$								
$(2104)3L$	$1.649241+0$	$-1.574276+0$	$-1.572703+0$	$(2104)3K$	$2.158730-1$	$2.0266261+0$	$-9.023294-1$								
$(2104)1K$	0.000000	$4.714042+0$	$-7.845749-1$	$(3004)3K$	$1.2044208+0$	$7.544148-1$	$-3.080709+0$								
$(2004)3I$	$-7.047615-1$	$1.696969-1$	$3.509519+0$	$(2104)3L$	$6.233546-1$	$-5.449630+0$	$5.138481+0$								
$(3004)3I$	$1.979485-1$	$-1.509607+0$	$2.583594+0$	$(3004)3K$	$7.174599-1$	$1.377200+0$	$1.972470+0$								
$(2104)3K$	$-1.121708+0$	$-1.112711+0$	$3.455395+0$	$(2104)3L$	$-1.511657+0$	$2.304436+0$	$3.995496+0$								
$(3004)3K$	$-5.441084-1$	$1.706522+0$	$-5.383146+0$	$(2104)3L$	$(2104)3L$	0.000000	$-1.266666+0$	$2.818392+0$							

TABLE I. (continued)

TABLE I. (continued)

		$J = 4.0$		$(1002)3F, (1102)3H, (2002)16, (2004)5D, (1004)5F, (2004)56, (2004)5I, (1004)3F, (2104)3F, (3004)3F.$		$(2004)36, (2104)3G, (3004)3G, (1104)3H, (2104)3H, (3004)3H, (2004)16, (2104)16, (2204)16,$	
		$(U_{TV}S_L)$	$(U_{V1}S_L)$	M^6	M^2	M^4	M^0
		$(U_{TV}S_L)$	$(U_{V1}S_L)$	M^6	M^2	M^4	M^0
(2204)1H	0.000000	-2.875048+0	-4.351904+0	(3004)3H	-1.341517+0	2.506408+0	-1.741705+0
(2004)51	9.09095-2	3.856748-2	2.200966-1	(2004)31	-3.195814-1	1.074956+0	-1.650738+0
(2004)36	0.000000	2.816897+0	-5.285138+0	(2104)31	1.107062+0	-5.032103+0	1.777071+0
(2104)36	-2.615755+0	2.337383+0	2.689523+0	(2104)3H	5.185102-1	-6.067538-1	6.433185+0
(3004)36	1.421613+0	1.881388+0	6.126337-1	(3004)3H	1.920221-2	1.027317+0	-1.256290+0
(1104)3H	-4.287636-1	1.442205+0	-2.214688+0	(2004)31	1.686653+0	2.208672+0	-4.719267+0
(2104)3H	-4.330875-1	5.986586-1	1.777412+0	(3004)31	8.534337-1	-2.984030-3	-1.796159+0
(3004)3H	4.531370-1	-1.651516+0	-1.380780+0	(3004)3H	-5.288885-1	2.168079+0	5.474108+0
(2004)31	-2.236066+0	2.735024+0	4.416435+0	(2004)31	3.377483-1	-1.702698-1	3.452536+0
(3004)31	2.112535+0	-1.429695+0	-1.675016+0	(3004)31	5.318156-1	3.867754-2	-4.920901-1
(2104)1H	0.000000	-3.013124+0	4.942341+0	(2004)31	-1.121211+0	2.699723-1	5.583325+0
(2204)1H	0.000000	4.845176-1	5.564523+0	(3004)31	3.149181-1	-2.401648+0	4.110263+0
(2004)31	-9.831165-2	9.750486-1	1.398875-1	(3004)31	6.060601-2	2.038566+0	6.636609-1
(2204)36	0.000000	-2.875048+0	-4.351904+0	(3004)3H	-1.341517+0	2.506408+0	-1.741705+0
(2004)51	9.09095-2	3.856748-2	2.200966-1	(2004)31	-3.195814-1	1.074956+0	-1.650738+0
(2004)36	0.000000	2.816897+0	-5.285138+0	(2104)3H	1.107062+0	-5.032103+0	1.777071+0
(2104)36	-2.615755+0	2.337383+0	2.689523+0	(2104)3H	5.185102-1	-6.067538-1	6.433185+0
(3004)36	1.421613+0	1.881388+0	6.126337-1	(3004)3H	1.920221-2	1.027317+0	-1.256290+0
(1104)3H	-4.287636-1	1.442205+0	-2.214688+0	(2004)31	1.686653+0	2.208672+0	-4.719267+0
(2104)3H	-4.330875-1	5.986586-1	1.777412+0	(3004)31	8.534337-1	-2.984030-3	-1.796159+0
(3004)3H	4.531370-1	-1.651516+0	-1.380780+0	(3004)3H	-5.288885-1	2.168079+0	5.474108+0
(2004)31	-2.236066+0	2.735024+0	4.416435+0	(2004)31	3.377483-1	-1.702698-1	3.452536+0
(3004)31	2.112535+0	-1.429695+0	-1.675016+0	(3004)31	5.318156-1	3.867754-2	-4.920901-1
(2104)1H	0.000000	-3.013124+0	4.942341+0	(2004)31	-1.121211+0	2.699723-1	5.583325+0
(2204)1H	0.000000	4.845176-1	5.564523+0	(3004)31	3.149181-1	-2.401648+0	4.110263+0
(2004)31	-9.831165-2	9.750486-1	1.398875-1	(3004)31	6.060601-2	2.038566+0	6.636609-1
(2204)36	0.000000	-2.875048+0	-4.351904+0	(3004)3H	-1.341517+0	2.506408+0	-1.741705+0
(2004)51	9.09095-2	3.856748-2	2.200966-1	(2004)31	-3.195814-1	1.074956+0	-1.650738+0
(2004)36	0.000000	2.816897+0	-5.285138+0	(2104)3H	1.107062+0	-5.032103+0	1.777071+0
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(3004)36	1.421613+0	1.881388+0	6.126337-1	(3004)3H	1.920221-2	1.027317+0	-1.256290+0
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(2204)1H	0.000000	4.845176-1	5.564523+0	(3004)31	3.149181-1	-2.401648+0	4.110263+0
(2004)31	-9.831165-2	9.750486-1	1.398875-1	(3004)31	6.060601-2	2.038566+0	6.636609-1
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(3004)3H	4.531370-1	-1.651516+0	-1.380780+0	(3004)3H	-5.288885-1	2.168079+0	5.474108+0
(2004)31	-2.236066+0	2.735024+0	4.416435+0	(2004)31	3.377483-1	-1.702698-1	3.452536+0
(3004)31	2.112535+0	-1.429695+0	-1.675016+0	(3004)31	5.318156-1	3.867754-2	-4.920901-1
(2104)1H	0.000000	-3.013124+0	4.942341+0	(2004)31	-1.121211+0	2.699723-1	5.583325+0
(2204)1H	0.000000	4.845176-1	5.564523+0	(3004)31	3.149181-1	-2.401648+0	4.110263+0
(2004)31	-9.831165-2	9.750486-1	1.398875-1	(3004)31	6.060601-2	2.038566+0	6.636609-1
(2204)36	0.000000	-2.875048+0	-4.351904+0	(3004)3H	-1.341517+0	2.506408+0	-1.741705+0
(2004)51	9.09095						

TABLE I. (continued)

TABLE I. (continued)

$J = 2.0$	(1102) 3P, (1002) 3F, (2002) 1D, (004) 5S, (2004) 5D, (1004) 5F, (2004) 1D, (2104) 1D, (2204) 1D, (3004) 3P, (3004) 3D.	(U _{Tv})SL (U _{T'} v')SL, M ⁰ , M ² , M ⁴ , (U _{Tv})SL (U _{T'} v')SL, M ⁰ , M ² , M ⁴	(U _{Tv})SL (U _{T'} v')SL, M ⁰ , M ² , M ⁴ , (U _{Tv})SL (U _{T'} v')SL, M ⁰ , M ² , M ⁴
(1102) 3P	(1102) 3P	-3.9999998-1 -7.9999996-1 -9.090964-2	(1004) 3F -7.628957-1 -3.190291+0
(1002) 3P	(1002) 3P	2.771280+0 9.237599-1 -8.397817+0	(2104) 3F 3.028959+0 1.139234+0
(1002) 3F	(1002) 3F	-5.33331-1 4.266664+0 -6.696964+0	(3004) 3F -1.658710+0 3.995983+0
(004) 5S	(2004) 5D	3.666059+0 -7.332117+0 6.331951+0	(2004) 1D 0.000000 2.422613+0
(2004) 3D	(2004) 3D	-3.666059+0 1.047445+0 6.331951+0	(2104) 1D 0.000000 1.621681+0
(2104) 3D	(2104) 3D	0.000000 2.514166+0 -3.076777+0	(2204) 1D 0.000000 4.001587+0
(2004) 1D	(2004) 1D	0.000000 4.984669+0 -1.317397+1	(1104) 3P -2.713843+0
(2104) 1D	(2104) 1D	0.000000 6.842694-1 -8.373927-1	(1004) 3P -2.676766+0
(2204) 1D	(2204) 1D	0.000000 -3.689787+0 -2.257737+0	(3004) 3P -3.806959-1
(2004) 5D	(2004) 5D	1.457142+0 -6.285711-1 -3.246751-1	(2004) 3D 9.758994-2
(1004) 5F	(1004) 5F	-2.962623+0 2.221967+0 5.049925+0	(2104) 3D -9.758993-2
(2004) 5G	(2004) 5G	-1.856922+0 3.455938+0 1.673191+0	(3004) 3D 2.217953-1
(1104) 3P	(1104) 3P	-6.831296-1 6.831298-1 -1.552567+0	(2104) 3D 2.093086+0
(3004) 3P	(3004) 3P	-3.171959+0 -4.819730+0 -1.966609+0	(1004) 3D -1.257307+0
(2004) 3D	(2004) 3D	1.428571-1 3.199998+0 -5.129867-1	(2004) 3D -1.11109-1
(2104) 3D	(2104) 3D	-1.392691+0 1.969461-1 4.108376+0	(1104) 3P -3.11109-1
(1004) 3F	(1004) 3F	4.507467-1 2.817179+0 -7.939323+0	(2004) 3D 3.11109-1
(2104) 3F	(2104) 3F	1.157994+0 -2.342306+0 -1.36461+0	(1004) 3P 3.11109-1
(3004) 3F	(3004) 3F	-1.078034+0 2.597082+0 1.087971-1	(2004) 3D 3.11109-1
(2004) 1D	(2004) 1D	0.000000 3.282743+0 -1.054092+1	(2104) 3D 3.11109-1
(2104) 1D	(2104) 1D	0.000000 5.372794-1 -2.375543-1	(1004) 3D 3.11109-1
(2204) 1D	(2204) 1D	0.000000 6.5088519+0 6.076369+0	(2004) 3D 3.11109-1
(1004) 5F	(1004) 5F	5.999996-1 -1.199999+0 1.363535+0	(2104) 3F 3.11109-1
(2004) 5G	(2004) 5G	-3.760697+0 2.279212-1 9.583043+0	(3004) 3F 3.11109-1
(1104) 3P	(1104) 3P	-2.529821+0 1.897365+0 4.312194+0	(2104) 3D 3.11109-1
(3004) 3P	(3004) 3P	-1.678093+0 -7.246311-1 5.287380+0	(1004) 3F 3.11109-1
(2004) 1D	(2004) 1D	0.000000 1.903004+0 -2.328851+0	(2104) 3F 3.11109-1
(2104) 1D	(2104) 1D	0.000000 -3.349741-1 1.332283+1	(3004) 3F 3.11109-1
(2204) 1D	(2204) 1D	0.000000 -1.413248+0 1.729500+0	(2104) 3F 3.11109-1
(2004) 5G	(2004) 5G	1.428572-1 -4.510820+0 -1.052734+0	(3004) 3F 3.11109-1
(2104) 3D	(2104) 3D	1.856922+0 -9.190826-1 1.833049+0	(3004) 3F 3.11109-1
		1.904761-1 -1.559595+0 -7.333067-1	
$J = 1.0$	(1102) 3P, (2004) 5D, (1004) 5F, (1104) 3P, (3004) 3P, (2004) 3D, (2104) 3D,	(U _{Tv})SL (U _{T'} v')SL, M ⁰ , M ² , M ⁴ , (U _{Tv})SL (U _{T'} v')SL, M ⁰ , M ² , M ⁴	(U _{Tv})SL (U _{T'} v')SL, M ⁰ , M ² , M ⁴ , (U _{Tv})SL (U _{T'} v')SL, M ⁰ , M ² , M ⁴
(1102) 3P	(1102) 3P	1.99999+0 3.999998+0 4.545452+0	(2104) 3D -1.228238+0 9.490933+0
(2004) 5D	(2004) 5D	-3.399998+0 1.466666+0 7.575751-1	(1104) 3P -1.886888+0 -1.555555+0
(1004) 5F	(1004) 5F	-2.771280+0 2.078460+0 4.723772+0	(3004) 3P -3.685137-1 2.144079+0
(1104) 3P	(1104) 3P	3.533331-1 -3.333332-1 7.575752-1	(2004) 3D -2.182177-1 2.182177-1
(3004) 3P	(3004) 3P	1.547757+0 2.351787+0 9.593536-1	(2104) 3D -1.181873+0 2.811425+0
(2004) 3D	(2004) 3D	2.182178-1 4.888078+0 -7.836002+0	(3004) 3P -7.777773-1 3.616159+0
(2104) 3D	(2104) 3D	-2.127371+0 3.008402-1 6.275647+0	(2004) 3D -1.013245+0 7.671712+0

TABLE I. (continued)

$J = .0$	(00)1S,	(1102)3P,	(2004)5D,	(1104)3P,	(3004)3P,	(2204)1S,
$(U^{\tau}v)SL$	$(U^{\tau}v')S'L'$	M^0	M^2	M^4	$(U^{\tau}v)SL$	$(U^{\tau}v')S'L'$
$(1102)3P$	$(1102)3P$	-3.999998+0	-7.99995+0	-9.090904+0	$(2204)1S$	0.000000
$(2004)5D$	$(2004)5D$	-6.799996+0	2.933332+0	1.515150+0	$(1104)3P$	3.777776+0
$(1104)3P$	$(1104)3P$	1.154700+0	-1.154700+0	2.624318+0	$(3004)3P$	7.370273-1
$(3004)3P$	$(3004)3P$	5.361589+0	8.146830+0	3.323298+0	$(3004)3P$	1.555555+0

a.The non-zero elements of the upper-half diagonal are listed in the table.

b.The states, $(U^{\tau}v)SL$, listed beside each J-value form the matrix grid for the J-block.

c.The state notation, $(U^{\tau}v)SL$, is similar in form to that used by Nielson and Koster (Ref. 7) in that the multiplicity is not placed as a superscript.

d.A given matrix element is formed from the sum of the three radial coefficients, listed to the right of the element, each multiplied by their appropriate radial integral.

e.Each table entry is to be multiplied by the power of ten indicated by its following single digit.