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SPIN-OTHER-ORBIT MATRIX ELEMENTS
FOR f^4 CONFIGURATIONS*

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ABSTRACT

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

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I. INTRODUCTION

In recent years, angular momentum techniques developed by Racah¹ have enabled researchers to derive closed form matrix expressions for various atomic interaction operators within and between complex configurations. However, the construction of an interaction matrix for a given representation generally involves a long and tedious computational process. Therefore, once it has been accomplished, it is desirable that other active researchers should not have to duplicate the effort. It is with this purpose that we present in this paper the Spin-Other-Orbit matrix elements for the f^4 configuration².

II. MATRIX ELEMENTS OF THE SPIN-OTHER-ORBIT INTERACTION

The matrix elements of the Spin-Other-Orbit interaction for f^n configurations³ can be written in tensor operator form as $(f^n_{\gamma SLJ} | H_{soo} | f^n_{\gamma' S' L' J'})$

$$= \delta(J, J') (-1)^{S'+L+J} \begin{Bmatrix} S & S' & 1 \\ L' & L & J \end{Bmatrix}$$

$$\times \{ (f^n_{\gamma SL} || H_{soo}^1 || f^n_{\gamma' S' L'}) + (f^n_{\gamma SL} || H_{soo}^2 || f^n_{\gamma' S' L'}) \} \quad (1)$$

The reduced matrix elements of H_{soo}^1 and H_{soo}^2 , occurring in the above expression, are given by $(f^n_{\gamma SL} || H_{soo}^1 || f^n_{\gamma' S' L'})$

$$= \left[-2nM^0(84)^{1/2} + 6(3)^{1/2} \sum_k \sum_k (-1)^{K+k} \right]$$

$$\begin{aligned}
 & \times \left(3 \left| \left| c^k \right| \right| 3 \right) \left(3 \left| \left| u^{(kk)} \right| \right| 3 \right) \left\{ \begin{matrix} K & 3 & 3 \\ 3 & k & 1 \end{matrix} \right\} \\
 & \times M^{(k-1)} \left. \right] (f^{n_{\gamma SL}} \left| \left| v^{11} \right| \right| f^{n_{\gamma' S' L'}}), \quad (2)
 \end{aligned}$$

where $k = 1, 3, 5, \dots, K = k \pm 1$, and ,

$$\begin{aligned}
 & (f^{n_{\gamma SL}} \left| \left| H_{SUO}^2 \right| \right| f^{n_{\gamma' S' L'}}) = -2(3)^{1/2} \sum_k \sum_k (-1)^{k+K+L+L'} \\
 & \times \left(3 \left| \left| c^k \right| \right| 3 \right) \left(3 \left| \left| u^{(kk)} \right| \right| 3 \right) M^{k-1} \\
 & \times \left[\sum_{\gamma'' L''} (f^{n_{\gamma SL}} \left| \left| u^k \right| \right| f^{n_{\gamma'' SL''}}) (f^{n_{\gamma'' SL''}} \left| \left| v^{1k} \right| \right| f^{n_{\gamma' S' L'}}) \right. \\
 & \left. \left\{ \begin{matrix} L & K & L'' \\ k & L' & 1 \end{matrix} \right\} + 2 \sum_{\gamma'' L''} (f^{n_{\gamma SL}} \left| \left| u^k \right| \right| f^{n_{\gamma'' SL''}}) \right. \\
 & \left. \times (f^{n_{\gamma'' SL''}} \left| \left| v^{1k} \right| \right| f^{n_{\gamma' S' L'}}) \left\{ \begin{matrix} L & k & L'' \\ K & L' & 1 \end{matrix} \right\} \right]. \quad (3)
 \end{aligned}$$

The term with $k = 1, K = 0$ should be omitted from the summation for the first term in braces of Eq. (3) since it is already included in Eq. (2). The reduced matrix elements occurring in Eqs. (2) and (3) have the following expressions:

$$\begin{aligned}
 & (f^{n_{\gamma SL}} \left| \left| u^{(k)} \right| \right| f^{n_{\gamma' S' L'}}) = n \{ (2L+1)(2L'+1) \}^{1/2} \\
 & \sum_{\bar{\gamma} \bar{S} \bar{L}} (f^{\bar{n}_{\gamma SL}} \left| \left| f^{\bar{n}-1}_{\bar{\gamma} \bar{S} \bar{L}} \right| \right| f^{\bar{n}_{\gamma' S' L'}}) (-1)^{\bar{L}+L+3+k} \\
 & \times \left\{ \begin{matrix} L & 3 & \bar{L} \\ 3 & L & k \end{matrix} \right\}, \quad (4)
 \end{aligned}$$

$$\begin{aligned}
& (f^n_{\gamma SL} || V^{(1k)} || f^n_{\gamma' S' L'}) = n(3/2)^{1/2} \{(2S+1)(2S'+1)(2L+1)(2L'+1)\}^{1/2} \\
& \times \sum_{\gamma SL} (f^n_{\gamma SL} \{ | f^{n-1}_{\gamma SL} \} (f^{n-1}_{\gamma SL} |) f^n_{\gamma' S' L'}) \\
& \times \left\{ \begin{matrix} S & S' & 1 \\ 1/2 & 1/2 & 3 \end{matrix} \right\} \left\{ \begin{matrix} L & L' & k \\ 3 & 3 & L \end{matrix} \right\} (-1)^{S+L+S'+L+3+3/2+k}, \quad (5) \\
& (3 || c^k || 3) = -7 \begin{pmatrix} 3 & k & 3 \\ 0 & 0 & 0 \end{pmatrix}. \quad (6)
\end{aligned}$$

Horie⁴ defined the matrix elements of the quantity $U^{(K,k)}$ as

$$\begin{aligned}
& (3 || U^{(k-1,k)} || 3) = 7(-1)^{(k-1)/2} \left\{ \frac{(K+1)(2k-1)(2k+1)}{3} \right\}^{1/2} \\
& \times \left\{ \frac{(k-1)!(k+1)!(6-k)!}{(7+k)!} \right\}^{1/2} \\
& \times \left(\frac{7+k}{2} \right)! / \left[\left(\frac{k-1}{2} \right)! \left(\frac{k+1}{2} \right)! \left(\frac{5-k}{2} \right)! \right], \quad (7)
\end{aligned}$$

and

$$(3 || U^{(k+1,k)} || 3) = - \left\{ \frac{k(2k+3)}{(k+1)(2k-1)} \right\}^{1/2} (3 || U^{(k-1,k)} || 3). \quad (8)$$

In Eqs. (4) thru (6),

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

are the Wigner 3-j and 6-j symbols. The coefficients $(f^n_{\gamma SL} \{ | f^{n-1}_{\gamma SL} \})$ are the coefficients of fractional parentage introduced by Racah¹. The matrix elements of the tensor operators $U^{(k)}$ and $V^{(11)}$ and appropriate fractional parentage coefficients have been tabulated by Neilson and Koster⁵.

The radial integral, $M^{(k-1)}$, is defined by Marvin⁶ as,

$$M^{(k-1)} = \left(\frac{1}{4c^2} \right) \int_{r_j >} \int_{r_1} P_{nl}^2(r_1) \left(\frac{r_1^{k-1}}{r_j^{k+2}} \right) P_{nl}^2(r_j) dr_1 dr_j ,$$

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

III. DISCUSSION OF TABLE

Table I presents a tabulation of the matrix elements of the Spin-Other-Orbit operator H_{soo} for f^4 configurations. The calculations were performed in single precision on the Univac 1108 computer. A comparison with the diagonal matrix elements of f^4 presented by Judd, et al⁷, indicates an accuracy of at least seven significant figures.

The matrix elements are tabulated in J-blocks. The states |(Urv)SL) labeling a given J-block are listed in parenthesis beside the J-value⁸. The matrices of H_{soo} 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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⁸The state notation may be related to that used by Nielson and Koster⁵ through the use of their tables presented on pages 2 and 3.

TABEL I. SPIN-OTHER-ORBIT INTERACTION OF f^4 ELECTRONS FOR VARIOUS J LEVELS. ^a

J = 10.0 ^b		(3004)3M, (2204)1M,C		(U _T V)SL (U' T' V')S' L'°		M ⁰	M ²	M ⁴	M ⁶	M ⁸
(3004)3M	(3004)3M ^d	-4.659998+1 ^e	3.975756+0	3.637422+0	(2204)1M	1.686549+0	-1.763208+0	-1.730239+0		
J = 9.0		(2104)3L, (3004)3M,		(U _T V)SL (U' T' V')S' L'°		M ⁰	M ²	M ⁴	M ⁶	
(2104)3L	(2104)3L	-4.077776+1	5.478112+0	2.355841+0	(3004)3M	5.177775+0	-4.417506+1	-4.041580+1		
(3004)3M	(3004)3M	-2.4046521+0	3.4632269+1	1.060889+0						
J = 8.0		(2004)5I, (2104)3K, (3004)3K, (2104)3L, (3004)3M, (2104)3L, (2204)1L,		(U _T V)SL (U' T' V')S' L'°		M ⁰	M ²	M ⁴	M ⁶	
(2004)5I	(2004)5I	-6.599997+1	1.090908+0	-7.438007+1	(2104)3L	2.654843+1	-3.998680+1	-6.619118+1		
(2104)3K	(2104)3K	-4.695781+0	2.344391+0	1.464989+0	(2204)1L	4.8333869+0	-2.887764+0	-3.011688+0		
(3004)3K	(3004)3K	3.967462+0	-3.664489+0	-4.055231+0	(2104)3L	5.097219+0	-6.847640+1	-2.5944802+1		
(2104)3K	(2104)3K	-3.585276+1	-1.774494+0	-1.759014+0	(3004)3M	-2.3493308+0	3.274791+1	1.003148+0		
(3004)3K	(3004)3K	-3.206849+1	-5.963924+0	-6.780681+0	(2104)3L	-4.831892+0	-4.981886+0	-6.237191+1		
(2104)3K	(2104)3K	4.163457+0	-1.100279+0	-6.072308+1	(2204)1L	-9.189340+1	-3.090967+0	-1.536429+0		
(2104)3L	(2104)3L	-5.568512+0	3.123123+0	7.297739+1	(3004)3M	5.177776+1	-4.417507+0	-4.041580+0		
(2204)1L	(2204)1L	2.135414+0	7.980845+1	-1.885476+1	(2104)3L	-1.993452+0	-1.449784+0	1.089071+1		
(3004)3K	(3004)3K	-3.662220+1	1.397779+0	-2.041815+0	(2204)1L	3.425778+0	-2.565045+0	1.030258+0		
(2104)3L	(2104)3L	-2.348342+0	2.117776+0	-5.135549+2						
J = 7.0		(2004)5I, (2004)3I, (2104)3I, (2104)3K, (3004)3K, (2104)3L, (2104)3K,		(U _T V)SL (U' T' V')S' L'°		M ⁰	M ²	M ⁴	M ⁶	
(2004)5I	(2004)5I	-2.199999+1	3.636362+1	-2.479336+1	(3004)3K	9.424237+1	-7.044378+1	-2.364214+0		
(2004)3I	(2004)3I	1.309306+0	1.375433+0	2.631191+1	(2104)3K	2.138088+0	-6.422773+1	-4.419805+1		
(2104)3K	(2104)3K	-5.039513+1	-5.909987+0	-4.935491+0	(2104)3K	5.121822+0	2.534991+1	2.512877+1		
(3004)3K	(3004)3K	2.597314+0	1.534764+0	9.590475+1	(3004)3K	4.581212+2	6.519891+1	9.686486+1		
(2004)3I	(2004)3I	-3.128570+1	8.225107+1	1.455946+0	(2104)3L	3.908955+0	-1.033022+0	-5.701123+1		
(2104)3K	(2104)3K	2.309400+0	-9.647493+1	3.180984+2	(3004)3K	-1.844100+0	-1.806848+0	-3.499768+1		
(2104)3K	(2104)3K	-3.409113+0	-4.340872+0	-4.045312+0	(2104)3L	-2.204794+0	-1.997113+1	2.916879+1		
(3004)3K	(3004)3K	6.030537+0	-7.312489+0	-3.118477+0	(2104)3L	1.322335+0	1.536046+0	-2.797481+2		
(2104)3K	(2104)3K	-7.530002+0	4.825485+1	-1.475740+0	(2104)3L	4.587498+1	-3.162874+0	-2.650322+0		
(3004)3I	(3004)3I	-3.047617+1	-3.670933+0	-5.275933+0	(2104)3K	5.926134+0	3.6468760+0	-7.769039+1		
(2104)3K	(2104)3K	-5.600000+0	2.274173+1	-2.058344+0						

TABLE I. (continued)

J = 4.0		(1102)JM, (2002)11, (2004)56, (2004)51, (1104)3M, (2104)3M, (3004)3M, (2004)31, (3004)31, (2104)3K, (3004)3K, (3004)31, (2204)11, (2204)11,		M ²		M ²		M ⁰		M ²		M ⁰		M ²	
(U'V'S'L)		(U'V'S'L)		(U'V'S'L)		(U'V'S'L)		(U'V'S'L)		(U'V'S'L)		(U'V'S'L)		(U'V'S'L)	
(1102)3M	(1102)3M	(2002)11	(2002)11	(2004)56	(2004)56	(2004)51	(2004)51	(1104)3M	(1104)3M	(2104)3M	(2104)3M	(3004)3M	(3004)3M	(2004)31	(2004)31
4.946644	4.946644	9.797942	9.797942	0.417155	2.377777	2.020202	2.020202	1.410776	1.410776	4.621322	4.621322	3.720424	3.720424	4.621322	4.621322
-5.372703	-5.372703	-0.494988	-0.494988	-1.911688	-1.911688	-3.032269	-3.032269	-1.750743	-1.750743	-2.086688	-2.086688	-2.395023	-2.395023	-2.086688	-2.086688
2.659080	2.659080	2.659080	2.659080	-1.093546	-1.093546	-1.750743	-1.750743	-4.943378	-4.943378	2.190356	2.190356	7.395023	7.395023	2.190356	2.190356
-1.075501	-1.075501	5.995800	5.995800	2.689041	2.689041	2.981422	2.981422	2.981422	2.981422	-2.320475	-2.320475	1.675900	1.675900	2.981422	2.981422
-2.517744	-2.517744	4.232720	4.232720	-7.086070	-7.086070	-5.629480	-5.629480	3.162116	3.162116	2.530598	2.530598	2.629835	2.629835	2.530598	2.530598
-6.374235	-6.374235	-7.032031	-7.032031	-9.310805	-9.310805	-1.419026	-1.419026	1.419026	1.419026	-2.854705	-2.854705	2.540880	2.540880	-2.854705	-2.854705
1.733189	1.733189	9.505315	9.505315	-2.780842	-2.780842	4.054624	4.054624	4.054624	4.054624	-2.367221	-2.367221	2.756902	2.756902	-2.367221	-2.367221
-5.733769	-5.733769	-2.095674	-2.095674	1.153816	1.153816	1.120527	1.120527	1.120527	1.120527	-3.192695	-3.192695	5.440662	5.440662	-3.192695	-3.192695
7.856937	7.856937	4.824456	4.824456	4.635469	4.635469	7.578089	7.578089	7.578089	7.578089	1.299315	1.299315	-1.945072	-1.945072	1.299315	1.299315
1.825743	1.825743	1.825743	1.825743	-2.047043	-2.047043	-5.680343	-5.680343	-3.272222	-3.272222	5.214282	5.214282	-1.370851	-1.370851	5.214282	5.214282
-1.475730	-1.475730	-7.007822	-7.007822	7.975228	7.975228	8.543386	8.543386	8.543386	8.543386	-3.849000	-3.849000	1.607915	1.607915	-3.849000	-3.849000
-5.282902	-5.282902	1.741364	1.741364	1.044352	1.044352	0.628111	0.628111	0.628111	0.628111	-5.079362	-5.079362	6.118322	6.118322	-5.079362	-5.079362
1.059393	1.059393	-1.084909	-1.084909	-2.639297	-2.639297	-2.639297	-2.639297	-2.639297	-2.639297	-6.951918	-6.951918	2.115573	2.115573	-6.951918	-6.951918
2.077325	2.077325	2.896405	2.896405	-7.036731	-7.036731	8.237673	8.237673	8.237673	8.237673	5.079362	5.079362	-4.714457	-4.714457	5.079362	5.079362
2.681544	2.681544	1.449999	1.449999	-2.727271	-2.727271	1.859502	1.859502	1.859502	1.859502	-5.209458	-5.209458	2.115573	2.115573	-5.209458	-5.209458
1.449999	1.449999	-1.329539	-1.329539	-1.698056	-1.698056	6.931786	6.931786	6.931786	6.931786	8.766996	8.766996	-6.553107	-6.553107	8.766996	8.766996
2.207566	2.207566	2.207566	2.207566	-1.280778	-1.280778	9.843356	9.843356	9.843356	9.843356	-4.715441	-4.715441	4.144573	4.144573	-4.715441	-4.715441
-3.108293	-3.108293	1.401528	1.401528	1.472314	1.472314	2.814522	2.814522	2.814522	2.814522	4.077458	4.077458	2.020202	2.020202	4.077458	4.077458
-5.394474	-5.394474	-1.632614	-1.632614	-6.322633	-6.322633	-5.283031	-5.283031	-3.010013	-3.010013	3.664970	3.664970	6.815913	6.815913	3.664970	3.664970
1.379394	1.379394	1.379394	1.379394	8.150903	8.150903	5.093357	5.093357	5.093357	5.093357	1.234664	1.234664	1.598737	1.598737	5.093357	5.093357
-2.683147	-2.683147	-1.701458	-1.701458	-4.484489	-4.484489	-1.409910	-1.409910	-1.409910	-1.409910	2.240877	2.240877	1.889375	1.889375	-1.409910	-1.409910
-9.493474	-9.493474	-6.778676	-6.778676	4.222585	4.222585	4.222585	4.222585	4.222585	4.222585	-6.058214	-6.058214	-2.143094	-2.143094	-6.058214	-6.058214
1.538118	1.538118	5.551104	5.551104	-1.091305	-1.091305	-1.091305	-1.091305	-1.091305	-1.091305	-3.362863	-3.362863	1.704591	1.704591	-3.362863	-3.362863

J = 5.0		(1102)JM, (1004)5F, (2004)56, (2004)51, (2004)36, (1104)3M, (2104)3M, (3004)3M, (2004)31, (3004)31, (2104)3K, (3004)3K, (3004)31, (2204)1M, (2204)1M,		M ²		M ²		M ⁰		M ²		M ⁰		M ²	
(U'V'S'L)		(U'V'S'L)		(U'V'S'L)		(U'V'S'L)		(U'V'S'L)		(U'V'S'L)		(U'V'S'L)		(U'V'S'L)	
(1102)3M	(1102)3M	(2004)51	(2004)51	(2004)36	(2004)36	(1104)3M	(1104)3M	(2104)3M	(2104)3M	(3004)3M	(3004)3M	(2004)31	(2004)31	(2004)31	(2004)31
4.946644	4.946644	4.946644	4.946644	-4.755553	-4.755553	-2.404039	-2.404039	1.410776	1.410776	4.621322	4.621322	3.720424	3.720424	4.621322	4.621322
-5.372703	-5.372703	4.287638	4.287638	-3.053314	-3.053314	-2.822289	-2.822289	-1.750743	-1.750743	-2.086688	-2.086688	-2.395023	-2.395023	-2.086688	-2.086688
2.659080	2.659080	-1.075501	-1.075501	-1.578979	-1.578979	-7.952175	-7.952175	-4.943378	-4.943378	2.190356	2.190356	7.395023	7.395023	2.190356	2.190356
-1.075501	-1.075501	5.995800	5.995800	2.689041	2.689041	2.981422	2.981422	2.981422	2.981422	-2.320475	-2.320475	1.675900	1.675900	2.981422	2.981422
-2.517744	-2.517744	4.232720	4.232720	-7.086070	-7.086070	-5.629480	-5.629480	3.162116	3.162116	2.530598	2.530598	2.629835	2.629835	2.530598	2.530598
-6.374235	-6.374235	-7.032031	-7.032031	-9.310805	-9.310805	-1.419026	-1.419026	1.419026	1.419026	-2.854705	-2.854705	2.540880	2.540880	-2.854705	-2.854705
1.733189	1.733189	9.505315	9.505315	-2.780842	-2.780842	4.054624	4.054624	4.054624	4.054624	-2.367221	-2.367221	2.756902	2.756902	-2.367221	-2.367221
-5.733769	-5.733769	-2.095674	-2.095674	1.153816	1.153816	1.120527	1.120527	1.120527	1.120527	-3.192695	-3.192695	5.440662	5.440662	-3.192695	-3.192695
7.856937	7.856937	4.824456	4.824456	4.635469	4.635469	7.578089	7.578089	7.578089	7.578089	1.299315	1.299315	-1.945072	-1.945072	1.299315	1.299315
1.825743	1.825743	1.825743	1.825743	-2.047043	-2.047043	-5.680343	-5.680343	-3.272222	-3.272222	5.214282	5.214282	-1.370851	-1.370851	5.214282	5.214282
-1.475730	-1.475730	-7.007822	-7.007822	7.975228	7.975228	8.543386	8.543386	8.543386	8.543386	-3.849000	-3.849000	1.607915	1.607915	-3.849000	-3.849000
-5.282902	-5.282902	1.741364	1.741364	1.044352	1.044352	0.628111	0.628111	0.628111	0.628111	-5.079362	-5.079362	6.118322	6.118322	-5.079362	-5.079362
1.059393	1.059393	-1.084909	-1.084909	-2.639297	-2.639297	-2.639297	-2.639297	-2.639297	-2.639297	-6.951918	-6.951918	2.115573	2.115573	-6.951918	-6.951918
2.077325	2.077325	2.896405	2.896405	-7.036731	-7.036731	8.237673	8.237673	8.237673	8.237673	5.079362	5.079362	-4.714457	-4.714457	5.079362	5.079362
2.681544	2.681544	1.449999	1.449999	-2.727271	-2.727271	1.859502	1.859502	1.859502	1.859502	-5.209458	-5.209458	2.115573	2.115573	-5.209458	-5.209458
1.449999	1.449999	-1.329539	-1.329539	-1.698056	-1.698056	6.931786	6.931786	6.931786	6.931786	8.766996	8.766996	-6.553107	-6.553107	8.766996	8.766996
2.207566	2.207566	2.207566	2.207566	-1.280778	-1.280778	9.843356	9.843356	9.843356	9.843356	-4.715441	-4.715441	4.144573	4.144573	-4.715441	-4.715441
-3.108293	-3.108293	1.401528	1.401528	1.472314	1.472314	2.814522	2.814522	2.814522	2.814522	4.077458	4.077458	2.020202	2.020202	4.077458	4.077458
-5.394474	-5.394474	-1.632614	-1.632614	-6.322633	-6.322633	-5.283031	-5.283031	-3.010013	-3.010013	3.664970	3.664970	6.815913	6.815913	3.664970	3.664970
1.379394	1.379394	1.379394	1.379394	8.150903	8.150903	5.093357	5.093357	5.093357	5.093357	1.234664	1.234664	1.598737	1.598737	5.093357	5.093357
-2.683147	-2.683147	-1.701458	-1.701458	-4.484489	-4.484489	-1.409910	-1.409910	-1.409910	-1.409910	2.240877	2.240877	1.889375	1.889375	-1.409910	-1.409910
-9.493474	-9.493474	-6.778676	-6.778676	4.222585	4.222585	4.222585	4.222585	4.222585	4.222585	-6.058214	-6.058214	-2.143094	-2.143094	-6.058214	-6.058214
1.538118	1.538118	5.551104	5.551104	-1.091305	-1.091305	-1.091305	-1.091305	-1.091305	-1.091305	-3.362863	-3.362863	1.704591	1.704591	-3.362863	-3.362863

TABLE I. (continued)

	M ⁰	M ¹	M ²	M ³	M ⁴	M ⁵	M ⁶	M ⁷	M ⁸	M ⁹
(2004)3F	-2.657390-1	-1.191799+0	-1.321374+0	(3004)3F	3.238146+0	8.341479+0	1.014713+1			
(2004)3G	4.025936+0	1.030562+0	1.488492+0	(2104)1F	-6.332019+0	-6.8870769+0	-9.155843+0			
(2104)3G	3.776737+0	1.972625+0	1.004786+0	(1004)3F	3.032129+0	1.469135-1	-1.332767-2			
(3004)3G	3.829707-1	1.717585+0	1.904303+0	(2104)3F	-6.422614-1	2.656265+1	4.760767-1			
(2104)1F	6.427371+0	-1.603097+0	-1.791055+0	(3004)3F	2.214491+2	-6.455579-1	-2.284195-1			
(1004)5F	2.721343+0	-4.082015+0	-6.803357+0	(2004)3G	3.416498+0	1.258506+0	-7.132358-1			
(2004)3D	-1.049046-1	1.520419+0	4.802149+0	(2104)3G	3.082021+0	2.250169+0	2.250169+0			
(2104)3D	-5.982974+0	-9.562225-1	-3.102330+0	(3004)3G	6.063702-1	9.303479-1	2.765020-1			
(1004)3F	1.461462+0	-1.954215+0	-2.233789-1	(2104)1F	-4.449718+0	1.176104+0	1.900017+0			
(2104)3F	-8.631181-1	-9.677384-1	-4.291813+0	(2104)3F	6.130886+0	-1.404040+0	-9.9125340-1			
(3004)3F	-4.519798+0	1.868791+0	1.859915+0	(3004)3F	1.241266+0	2.797087-1	1.179276+0			
(1004)5F	1.462499+1	-1.499999+0	-1.704544-1	(2004)3G	-1.051602+0	-2.949594+0	-6.302622+0			
(2004)5G	4.071074+0	5.263611+0	4.018737+0	(2104)3G	-6.336548+2	1.142119+0	-8.006238-1			
(2004)3D	-5.414417+0	-9.983417+0	-2.976311+0	(3004)3G	5.068421+0	-4.818837+0	-6.519295+0			
(2104)3D	-2.899636+0	2.568059+0	3.021112+0	(2104)1F	-5.677276+0	-4.198911-1	3.741641+0			
(1004)3F	1.041667+0	-7.222220-1	6.944447-7	(3004)3F	5.225923+0	-2.258136-1	2.166457-1			
(2104)3F	-7.493051+0	1.183966+0	2.373831+0	(2004)3G	-3.4628015+0	3.751914+0	2.757892+0			
(3004)3F	-9.765213-1	2.234623+0	-1.0088347+0	(2104)3G	3.191424+0	3.0843350+0	5.072866+0			
(2004)3G	1.809905+0	-1.979792+0	-1.470859+0	(3004)3G	1.734721+0	1.555992+0	4.045476+0			
(2104)3G	2.750772+0	-1.367125+0	1.027373+0	(2104)1F	5.374835-1	5.049087-1	-1.648670+0			
(3004)3G	-4.787133-1	-3.9578261-1	3.582657-1	(2004)3G	2.456546+1	7.828281-1	9.798463-1			
(2004)5G	3.657498+1	-9.269693+0	-9.138081+0	(2104)3G	-2.4536249+0	-4.533950+0	-6.072811+0			
(1004)3F	-2.141084+0	-3.063129+0	1.117354-1	(3004)3G	-4.8841228+0	-1.198408+0	1.739404+0			
(2104)3F	-5.563930+0	-1.973092+0	-3.889844+0	(2104)1F	8.142885+0	8.495667+0	5.228254+0			
(3004)3F	-5.442004+0	1.410669+0	-7.428482-1	(2104)3G	2.835951+1	4.807405+0	1.412152+0			
(2004)3G	-7.441240-1	1.670860-1	-2.2322336+0	(3004)3G	-3.986808+0	1.8702399+0	2.303184+0			
(2104)3G	-2.325228+0	8.092260-1	4.358328+0	(2104)1F	-2.867065+0	-7.912831+0	-1.105358+1			
(3004)3G	3.483573+0	3.797586+0	4.745464+0	(3004)3G	2.336332-1	-8.138716+0	-7.691609+0			
(2004)3D	-8.542863+0	1.5555555+0	1.412698+0	(2104)1F	-2.581988-1	2.167305+0	-1.532833+0			

J = 2.0	(1102)3P, (1002)3F, (2004)3D, (1004)5F, (2004)5G, (1104)3P, (3004)3P, (2004)3D, (2104)3D, (1004)3F, (3004)3F, (2004)1D, (2104)1D, (2204)1D,	(UTV)SL	(U'T'V')S'L*	M ⁰	M ¹	M ²	M ³	M ⁴	M ⁵
(1102)3P	-6.999997+0	-6.7333330+0	-6.949492+0	(2004)5G	5.224998+1	-1.324242+1	-1.305440+1		
(2002)1D	-3.280976+0	2.658720+0	1.902759+0	(1004)3F	-2.730281+0	-3.887458+0	1.413354+1		
(104)5S	-8.944280-1	1.490711+0	-1.355192-1	(2104)3F	-7.037877+0	-2.495786+0	-4.931691+0		
(2004)5D	7.377804+0	-2.413725+0	-1.780278+0	(3004)3F	-6.883652+0	1.784370+0	-9.396369+1		
(1104)3P	1.666667-1	-1.144444+0	-1.247474+0	(1104)3P	-4.194442+0	1.733333+0	5.916664+0		
(3004)3P	6.743803+0	-1.128992+0	-8.949198-1	(3004)3P	-1.289809-1	8.844328-1	-9.433645-1		
(2004)3D	2.283605+0	4.293959-1	8.760532-1	(2004)3D	-1.177911+1	-2.020112+0	4.923859+1		
(2104)3D	9.513895-1	-4.266838+0	4.730738+0	(2104)3D	-7.135422-1	-1.075599+1	-6.949773+0		
(2004)1D	3.175562+0	8.712993-1	2.291149+2	(2004)1D	-1.071534+1	-2.921480-1	1.114958+0		
(2204)1D	-6.428607+0	9.052759-1	-2.448099-1	(2104)1D	9.710077-1	-1.088706+0	-3.5044188+0		
(1002)3F	2.504666+1	7.011110-1	-1.010101+0	(2004)1D	3.214304+0	-7.792249+1	-1.2224049-1		
(2002)1D	5.976754+0	1.567672+0	5.062276+0	(3004)3P	-5.605553+0	-5.587876+0	-6.321622+0		
(2004)5F	1.735383+0	3.080115-1	2.629367-1	(2004)3D	-1.132884+0	-1.085764+0	1.713307+0		
(1004)5F	-3.651484+0	8.520126-1	2.213020-1	(2104)3D	-7.529940+0	4.101458+0	6.739373+0		
(2004)5G	-5.408327+0	1.622888+0	2.118455+0	(2004)1D	1.301592+0	4.867671+0	2.838751+0		
(2004)3D	3.493304+0	-2.441555+0	-2.339112+0	(2104)1D	4.098779-1	9.812224-1	-1.705001+0		
(2104)3D	-2.868489+0	7.212835-2	-7.288490-1	(2204)1D	-4.047621+0	-1.374429+1	-1.667213+1		
(1004)3F	2.577777+0	1.629629-1	-2.693601-1	(2004)3D	4.271475+0	-7.777775-1	-7.063489-1		
(2104)3F	5.138093+0	-1.159098+0	2.280449-1	(2104)3D	-5.158115-1	2.598595-1	1.903743+0		
(3004)3F	-1.062956+0	-4.767197+0	-5.285497+0	(1004)3F	3.831365+0	-1.314684+0	2.219596+1		

TABLE I. (continued)

(2004)1D	2.879294+0	-6.366753-1	-1.377879+0	(2104)3F	3.859980-1	3.678679+0	6.887886+0
(2104)1D	4.410146+0	-3.223234+0	-3.580802+0	(3004)3F	4.716400+0	3.013594+0	9.864556-1
(1104)3P	-2.856089+0	9.836635-1	8.156723-1	(2104)1D	1.307444+0	2.467579+0	5.866193+0
(3004)3P	2.470285+0	3.702110+0	4.414329+0	(2104)1D	1.307698+1	6.761508+0	3.230042+0
(2004)3D	2.760306+2	-3.744754+0	-3.508877+0	(2204)1D	5.535598-1	-2.482631+0	3.483355+0
(2104)3D	1.061425+1	1.599189+0	1.752362+0	(2104)3D	3.984125+0	8.161013-1	9.565783-1
(1004)3F	-1.328167+0	-8.201249-1	-1.124950+0	(1004)3F	-2.186665-1	-2.575197+0	-2.386974+0
(2104)3F	-1.118729+0	-5.017329+0	-5.562824+0	(2104)3F	3.836884+0	-5.632820+0	-2.499508+2
(3004)3F	6.379067+0	-2.102685+0	-1.041839+0	(3004)3F	2.709227+0	-6.778982+0	8.489898+0
(1104)3P	-1.311826+1	-9.938075-1	1.174500+0	(2004)1D	-4.815962+0	-2.106024+0	-7.788387-1
(3004)3P	-1.088261-1	-9.108884+0	-4.916889+0	(2104)1D	2.293967+0	-4.034410+0	-6.498551+0
(2004)5D	1.829999+1	7.799994+0	9.136359+0	(2204)1D	1.362749-1	4.583861-1	2.278056-1
(1004)5F	2.221967+0	-3.332951+0	-5.554918+0	(1004)3F	1.328517+1	5.876530-1	-5.331049+2
(1104)3P	-1.320717+0	-2.011770+0	-6.8031295-1	(2104)3F	-2.569045+0	1.062250+0	1.904307+0
(3004)3P	-3.776142+0	-7.765121+0	-7.883086+0	(3004)3F	8.857964-2	-2.582223+0	-1.313678+0
(2004)3D	-1.000001-1	1.422221+0	-4.510099+0	(2004)1D	1.345571+1	3.066178+0	-2.597362+0
(2104)3D	-5.596559+0	-8.994464-1	-2.901973+0	(2104)1D	-1.083850+0	3.570926+0	3.151059+0
(1004)3F	6.535858+0	-8.739517-1	-1.001664-1	(2104)3F	2.455555+1	-5.616159+0	-3.650136+0
(2104)3F	-3.859981-1	-4.327857+0	-1.919357+0	(3004)3F	4.765063+0	3.118835+0	4.717105+0
(3004)3F	-2.021315+0	8.357487-1	8.317794-1	(2004)1D	-5.798008-1	5.354604+0	3.008920+0
(1004)5F	2.924999+1	-2.999979+0	-3.409089-1	(2104)1D	7.492146+0	1.086989+1	1.083334+1
(2004)5D	2.820523+0	3.646737+0	2.784262+0	(2204)1D	-1.019803+0	1.715124+0	1.324188+0
(2004)3D	-8.270658+0	-6.612296+0	-4.526228+0	(3004)3F	2.090369+1	-9.032546-1	8.665828-1
(2104)3D	-4.429267+0	3.922774+0	4.614826+0	(2004)1D	2.151960+0	3.960007-2	-1.144648+0
(1004)3F	7.607262+1	-5.274364-1	5.071507-2	(2104)1D	4.875592-1	-1.898526+0	3.399518+0
(2104)3F	-5.472151+0	8.646467-1	1.733681+0	(2204)1D	7.613343+0	-2.748570+0	-1.413875+0
(3004)3F	-7.277562-1	1.631938+0	-7.363925-1				

J = 1.0 (1102)3P, (2004)5D, (1004)5F, (1104)3P, (3004)3P, (2004)3D, (2104)3D,

UTVSL (U'T'V'S'L'	M ⁰	M ¹	M ²	M ³	M ⁴	M ⁵	M ⁶	M ⁷	M ⁸
(1102)3P	6.999997+0	8.733330+0	9.969692+0	(2004)3D	-1.012945+1	-9.323120+0	-5.543476+0		
(2004)5D	1.080000+1	-3.533332+0	-2.606059+0	(2104)3D	-5.424723+0	4.804339+0	5.651984+0		
(1104)3P	-1.646667-1	1.144444+0	1.247474+0	(1104)3P	4.194442+0	-1.733332+0	-5.916664+0		
(3004)3P	-6.743803+0	1.128992+0	8.969197-1	(3004)3P	1.289807-1	-8.844328-1	9.433645-1		
(2004)3D	-1.702099+0	-3.200528-1	6.678786-1	(2004)3D	-8.779631+0	-1.505703+0	3.670028-1		
(2104)3D	7.091238-1	3.180313+0	3.526084+0	(2104)3D	-5.318429-1	-8.017039+0	-5.180055+0		
(2004)5D	3.049999+1	1.222726+1	1.522726+1	(3004)3P	5.605553+0	5.587876+0	6.321622+0		
(1004)5F	1.385640+0	-2.078460+0	-3.464100+0	(2004)3D	-8.443711-1	-8.092806-1	1.277024+0		
(1104)3P	-1.933332+0	-3.099999+0	-9.999992-1	(2104)3D	-5.612488+0	4.547758+0	5.023232+0		
(3004)3P	-5.527707+0	-1.136697+1	-1.153966+1	(2004)3D	1.281428+1	-2.333332+0	-2.119047+0		
(2004)3D	-6.546544+2	9.310625+1	2.952553+0	(2104)3D	-1.547435+0	7.795785-1	5.711229+0		
(2104)3D	-3.663808+0	-5.855643-1	-1.889987+0	(2104)3D	1.195237+1	2.448484+0	2.869735+0		
(1004)5F	3.899998+1	-3.999998+0	-4.545452-1						

J = 0.0 (00)1S, (1102)3P, (2004)5D, (1104)3P, (3004)3P, (2204)1S,

UTVSL (U'T'V'S'L'	M ⁰	M ¹	M ²	M ³	M ⁴	M ⁵	M ⁶	M ⁷	M ⁸
(1102)3P	1.699411+1	-2.683281+0	-1.219673+0	(2004)5D	3.655998+1	1.555999+1	1.827272+1		
(1104)3P	-4.173992+0	-1.590092+0	6.324230-1	(1104)3P	-2.237420+0	-3.579570+0	-1.154700+0		

TABLE I. (continued)

(3004)3P	1.977652+0	0.069470+0	9.033779+0	(3004)3P	-6.382846+0	-1.312545+1	-1.332405+1
(1102)3P	1.399999+1	1.746666+1	1.993930+1	(1104)3P	0.388884+0	-3.466665+0	-1.183333+1
(2004)5D	1.247076+1	-4.079940+0	-3.009218+0	(3004)3P	2.579617-1	-1.768866+0	1.086729+0
(1104)13P	-3.333333-1	2.288888+0	2.994940+0	(2204)1S	3.146427+0	-5.720773+0	-1.950263+0
(3004)3P	-1.348761+1	2.257984+0	1.793839+0	(3004)3P	1.121111+1	1.117575+1	1.264324+1
(2204)1S	-2.292853+0	-4.767311+0	-3.900527+0	(2204)1S	-9.803050+0	-2.943772+1	-3.709774+1

^aThe non-zero elements of the upper-half diagonal are listed in the table.

^bThe states, (Urv)SL, listed beside each J-value form the matrix grid for the J-block.

^cThe state notation, (Urv)SL, is similar in form to that used by Nielson and Koster (Ref.5) in that the multiplicity is not placed as a superscript.

^dA 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.

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