

Matrix elements for configuration d^5 in weak octahedral field using Racah methods

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Abstract—The matrix elements of the spin-orbit and crystal field interactions in a weak-cubic-field scheme have been calculated for the d^5 configuration. These matrices will be of use in the analysis of spectra of d^5 complexes having octahedral or near-octahedral symmetry.

1. INTRODUCTION

THE matrix elements of the weak cubic crystalline field (including spin-orbit interaction) in the $|SLJ\Gamma\rangle$ scheme were first reported for the d^2 configuration by LIEHR and BALLHAUSEN [1]. Since then the similar matrices for configurations d^3 and d^4 have been calculated by SCHONFELD [2] and DUNN and LI, [3], respectively. The matrices for the d^5 configuration have been calculated by LOW and ROSENGARTEN [4], even though the matrix elements were not given explicitly. Instead, Low and Rosengarten reported a few sets of eigenvalues by assigning numerical values for the parameters B , C , Dq and ζ . However, it is desirable that these matrices should be made available to spectroscopists so that eigenvalues can be obtained for different sets of parameters.

2. METHOD OF CALCULATION AND RESULTS

The matrix elements of the spin-orbit interaction

$$(d^n v' S' L' J' M' | \zeta_{nd} \sum_i \vec{l}_i \cdot \vec{s}_i | d^n v SLJM),$$

where v is RACAH's seniority number [5], have been evaluated by RACAH using irreducible tensor operator methods. These can be expressed in the form [5]

$$\begin{aligned} (d^n v' S' L' J' M' | \zeta_{nd} \sum_i \vec{l}_i \cdot \vec{s}_i | d^n v SLJM) \\ = (-1)^{S+L-J} (30)^{1/2} (d^n v' S' L' \| V^{(11)} \| d^n v SL) \\ W(S' L' S L; J 1) \delta_{J' J} \delta_{M' M} \zeta_{nd} \quad (1) \end{aligned}$$

The reduced matrix elements $(d^n v' S' L' \| V^{(11)} \| d^n v SL)$ in (1) are tabulated in numerous books [6] and the coefficients $W(abcd; ef)$ are the usual Racah coefficients.

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Table 1. Non-vanishing matrix elements of $(d^5v'S'L'J'\Gamma_6 | V_{oct} + V_{so} | d^5vSLJ\Gamma_6)$

$v'S'L'J'$	$vSLJ$	Dq	ζ_{nd}	$v'S'L'J'$	$vSLJ$	Dq	ζ_{nd}
${}^4G_{3\frac{1}{2}}$	${}^4F_{3\frac{1}{2}}$	$22(105)^{1/2}/63$	$2(105)^{1/2}/21$	${}^4F_{3\frac{1}{2}}$	${}^4D_{3\frac{1}{2}}$	$-20(21)^{1/2}/21$	$2(21)^{1/2}/7$
${}^4G_{3\frac{1}{2}}$	${}^4F_{4\frac{1}{2}}$	$-20(21)^{1/2}/63$	0	${}^4F_{3\frac{1}{2}}$	${}^2G_{3\frac{1}{2}}$	0	$(66)^{1/2}/12$
${}^4G_{3\frac{1}{2}}$	${}^4P_{\frac{1}{2}}$	$2(70)^{1/2}/3$	0	${}^4F_{3\frac{1}{2}}$	${}^2F_{3\frac{1}{2}}$	0	$-(30)^{1/2}/4$
${}^4G_{3\frac{1}{2}}$	${}^2G_{3\frac{1}{2}}$	0	$-(42)^{1/2}/12$	${}^4F_{4\frac{1}{2}}$	${}^4D_{\frac{1}{2}}$	$2(70)^{1/2}/7$	0
${}^4G_{3\frac{1}{2}}$	${}^2F_{3\frac{1}{2}}$	0	$-5(70)^{1/2}/28$	${}^4F_{4\frac{1}{2}}$	${}^4D_{3\frac{1}{2}}$	$-4(105)^{1/2}/21$	0
${}^4G_{4\frac{1}{2}}$	${}^4F_{3\frac{1}{2}}$	$4(165)^{1/2}/99$	0	${}^4F_{4\frac{1}{2}}$	${}^2G_{4\frac{1}{2}}$	0	$(66)^{1/2}/6$
${}^4G_{4\frac{1}{2}}$	${}^4F_{4\frac{1}{2}}$	$70(33)^{1/2}/99$	$(33)^{1/2}/6$	${}^4D_{\frac{1}{2}}$	${}^4P_{\frac{1}{2}}$	0	$(21)^{1/2}/6$
${}^4G_{4\frac{1}{2}}$	${}^4P_{\frac{1}{2}}$	$-2(110)^{1/2}/3$	0	${}^4D_{\frac{1}{2}}$	${}^2P_{\frac{1}{2}}$	0	$-(6)^{1/2}/3$
${}^4G_{4\frac{1}{2}}$	${}^2H_{4\frac{1}{2}}$	0	$2(5)^{1/2}/5$	${}^4D_{3\frac{1}{2}}$	${}^2D_{3\frac{1}{2}}$	0	$-2(14)^{1/2}/7$
${}^4G_{4\frac{1}{2}}$	${}^2G_{4\frac{1}{2}}$	0	$-(330)^{1/2}/30$	${}^4P_{\frac{1}{2}}$	${}^2S_{\frac{1}{2}}$	0	$-(21)^{1/2}/3$
${}^4G_{5\frac{1}{2}}$	${}^4F_{3\frac{1}{2}}$	$20(385)^{1/2}/77$	0	${}^5I_{5\frac{1}{2}}$	${}^2H_{4\frac{1}{2}}$	$-32(445)^{1/2}/143$	0
${}^4G_{5\frac{1}{2}}$	${}^4F_{4\frac{1}{2}}$	$20(77)^{1/2}/77$	0	${}^5I_{5\frac{1}{2}}$	${}^2H_{5\frac{1}{2}}$	$140(13)^{1/2}/143$	$(13)^{1/2}/2$
${}^4G_{5\frac{1}{2}}$	${}^2H_{5\frac{1}{2}}$	0	$(3)^{1/2}$	${}^5I_{5\frac{1}{2}}$	${}^2G_{5\frac{1}{2}}$	$25(6006)^{1/2}/1001$	0
${}^4F_{3\frac{1}{2}}$	${}^4D_{\frac{1}{2}}$	$10(14)^{1/2}/7$	0	${}^5I_{5\frac{1}{2}}$	${}^2G_{4\frac{1}{2}}$	$-2(30030)^{1/2}/1001$	0
${}^2I_{5\frac{1}{2}}$	${}^2F_{3\frac{1}{2}}$	$5(10010)^{1/2}/143$	0	${}^2G_{3\frac{1}{2}}$	${}^2F_{3\frac{1}{2}}$	$5(3)^{1/2}/3$	$-3(3)^{1/2}/4$
${}^2I_{5\frac{1}{2}}$	${}^2H_{4\frac{1}{2}}$	$-32(390)^{1/2}/143$	0	${}^2G_{3\frac{1}{2}}$	${}^2S_{\frac{1}{2}}$	$-16(35)^{1/2}/21$	0
${}^2I_{5\frac{1}{2}}$	${}^2H_{5\frac{1}{2}}$	$20(546)^{1/2}/143$	0	${}^2G_{4\frac{1}{2}}$	${}^2G_{3\frac{1}{2}}$	$10(33)^{1/2}/33$	0
${}^2I_{5\frac{1}{2}}$	${}^2G_{3\frac{1}{2}}$	$-10(143)^{1/2}/429$	0	${}^2G_{4\frac{1}{2}}$	${}^2G_{4\frac{1}{2}}$	$-14(165)^{1/2}/33$	$-(165)^{1/2}/15$
${}^2I_{5\frac{1}{2}}$	${}^2G_{4\frac{1}{2}}$	$32(715)^{1/2}/429$	0	${}^2G_{4\frac{1}{2}}$	${}^2F_{3\frac{1}{2}}$	$2(15)^{1/2}/3$	0
${}^2I_{5\frac{1}{2}}$	${}^2F_{3\frac{1}{2}}$	$10(2145)^{1/2}/143$	0	${}^2G_{4\frac{1}{2}}$	${}^2S_{\frac{1}{2}}$	$40(7)^{1/2}/21$	0
${}^2H_{4\frac{1}{2}}$	${}^2G_{3\frac{1}{2}}$	$-35(2)^{1/2}/33$	0	${}^2G_{5\frac{1}{2}}$	${}^2F_{5\frac{1}{2}}$	$35(11)^{1/2}/33$	$(11)^{1/2}/4$
${}^2H_{4\frac{1}{2}}$	${}^2G_{4\frac{1}{2}}$	$-14(10)^{1/2}/33$	$2(10)^{1/2}/5$	${}^2G_{5\frac{1}{2}}$	${}^2P_{\frac{1}{2}}$	$-5(154)^{1/2}/21$	0
${}^2H_{4\frac{1}{2}}$	${}^2F_{3\frac{1}{2}}$	$-(110)^{1/2}/11$	0	${}^2G_{4\frac{1}{2}}$	${}^2F_{3\frac{1}{2}}$	$14(55)^{1/2}/33$	0
${}^2H_{5\frac{1}{2}}$	${}^2G_{3\frac{1}{2}}$	$-15(70)^{1/2}/77$	0	${}^2G_{4\frac{1}{2}}$	${}^2P_{\frac{1}{2}}$	$-2(770)^{1/2}/21$	0
${}^2H_{5\frac{1}{2}}$	${}^2G_{4\frac{1}{2}}$	$-30(14)^{1/2}/77$	0	${}^2F_{3\frac{1}{2}}$	${}^2F_{3\frac{1}{2}}$	$-(5)^{1/2}$	$-(5)^{1/2}/4$
${}^2H_{5\frac{1}{2}}$	${}^2F_{3\frac{1}{2}}$	$25(154)^{1/2}/77$	0	${}^2F_{3\frac{1}{2}}$	${}^2P_{\frac{1}{2}}$	$3(70)^{1/2}/7$	0
${}^2G_{3\frac{1}{2}}$	${}^2G_{3\frac{1}{2}}$	$-13(165)^{1/2}/33$	$(165)^{1/2}/12$	${}^2P_{\frac{1}{2}}$	${}^2S_{\frac{1}{2}}$	0	$2(6)^{1/2}/3$
${}^2G_{3\frac{1}{2}}$	${}^2G_{4\frac{1}{2}}$	$10(33)^{1/2}/33$	0				

Table 2. Non-vanishing matrix elements of $(d^5v'S'L'J'\Gamma_7 | V_{oct} + V_{so} | d^5vSLJ\Gamma_7)$

$v'S'L'J'$	$vSLJ$	Dq	ζ_{nd}	$v'S'L'J'$	$vSLJ$	Dq	ζ_{nd}
${}^6S_{2\frac{1}{2}}$	${}^4P_{2\frac{1}{2}}$	0	$-(5)^{1/2}$	${}^4F_{2\frac{1}{2}}$	${}^4D_{2\frac{1}{2}}$	$10(70)^{1/2}/49$	$16(70)^{1/2}/105$
${}^4G_{2\frac{1}{2}}$	${}^4F_{2\frac{1}{2}}$	$-22(105)^{1/2}/49$	$(105)^{1/2}/14$	${}^4F_{2\frac{1}{2}}$	${}^4D_{3\frac{1}{2}}$	$-20(105)^{1/2}/49$	0
${}^4G_{2\frac{1}{2}}$	${}^4F_{3\frac{1}{2}}$	$100(21)^{1/2}/147$	0	${}^4F_{2\frac{1}{2}}$	${}^2F_{2\frac{1}{2}}$	0	$-5(2)^{1/2}$
${}^4G_{2\frac{1}{2}}$	${}^4P_{2\frac{1}{2}}$	$-2(30)^{1/2}/3$	0	${}^4F_{2\frac{1}{2}}$	${}^2D_{2\frac{1}{2}}$	0	$2(70)^{1/2}/15$
${}^4G_{2\frac{1}{2}}$	${}^2F_{2\frac{1}{2}}$	0	$-5(42)^{1/2}/14$	${}^4F_{2\frac{1}{2}}$	${}^2D_{2\frac{1}{2}}$	0	$2(5)^{1/2}/15$
${}^4G_{3\frac{1}{2}}$	${}^4F_{2\frac{1}{2}}$	$4(21)^{1/2}/49$	0	${}^4F_{3\frac{1}{2}}$	${}^4D_{2\frac{1}{2}}$	$-30(14)^{1/2}/49$	0
${}^4G_{3\frac{1}{2}}$	${}^4F_{3\frac{1}{2}}$	$-22(105)^{1/2}/49$	$2(105)^{1/2}/21$	${}^4F_{3\frac{1}{2}}$	${}^4D_{3\frac{1}{2}}$	$60(21)^{1/2}/49$	$2(21)^{1/2}/7$
${}^4G_{3\frac{1}{2}}$	${}^4P_{2\frac{1}{2}}$	$-2(6)^{1/2}$	0	${}^4F_{3\frac{1}{2}}$	${}^2G_{3\frac{1}{2}}$	0	$(66)^{1/2}/12$
${}^4G_{3\frac{1}{2}}$	${}^2G_{3\frac{1}{2}}$	0	$-(42)^{1/2}/12$	${}^4F_{3\frac{1}{2}}$	${}^2F_{3\frac{1}{2}}$	0	$-(30)^{1/2}/4$
${}^4G_{3\frac{1}{2}}$	${}^2F_{3\frac{1}{2}}$	0	$-5(70)^{1/2}/28$	${}^4D_{2\frac{1}{2}}$	${}^4P_{2\frac{1}{2}}$	0	$7(5)^{1/2}/10$
${}^4G_{5\frac{1}{2}}$	${}^4F_{2\frac{1}{2}}$	$-4(21)^{1/2}/7$	0	${}^4D_{2\frac{1}{2}}$	${}^2F_{2\frac{1}{2}}$	0	$-4(7)^{1/2}/21$
${}^4G_{5\frac{1}{2}}$	${}^4F_{3\frac{1}{2}}$	$-4(105)^{1/2}/21$	0	${}^4D_{2\frac{1}{2}}$	${}^2D_{2\frac{1}{2}}$	0	$-2(7)^{1/2}/3$
${}^4G_{5\frac{1}{2}}$	${}^4P_{2\frac{1}{2}}$	$-8(6)^{1/2}/3$	0	${}^4D_{3\frac{1}{2}}$	${}^2F_{3\frac{1}{2}}$	0	$-2(14)^{1/2}/7$
${}^4G_{5\frac{1}{2}}$	${}^2H_{5\frac{1}{2}}$	0	$(3)^{1/2}$	${}^4P_{2\frac{1}{2}}$	${}^2D_{2\frac{1}{2}}$	0	$4(5)^{1/2}/5$
${}^4P_{2\frac{1}{2}}$	${}^5D_{2\frac{1}{2}}$	0	$(70)^{1/2}/5$	${}^5I_{6\frac{1}{2}}$	${}^2F_{3\frac{1}{2}}$	$-25(66)^{1/2}/154$	0
${}^2I_{5\frac{1}{2}}$	${}^2H_{5\frac{1}{2}}$	$-20(13)^{1/2}/39$	$(13)^{1/2}/2$	${}^5I_{6\frac{1}{2}}$	${}^2D_{2\frac{1}{2}}$	$85(22)^{1/2}/462$	0
${}^2I_{5\frac{1}{2}}$	${}^2G_{3\frac{1}{2}}$	$-5(182)^{1/2}/91$	0	${}^2H_{5\frac{1}{2}}$	${}^2G_{5\frac{1}{2}}$	$(2310)^{1/2}/77$	0
${}^2I_{5\frac{1}{2}}$	${}^2F_{2\frac{1}{2}}$	$10(910)^{1/2}/39$	0	${}^2H_{5\frac{1}{2}}$	${}^2F_{2\frac{1}{2}}$	$-10(14)^{1/2}/21$	0

Table 2 (cont.)

$v'S'L'J'$	$vSLJ$	Dq	ζ_{nd}	$v'S'L'J'$	$vSLJ$	Dq	ζ_{nd}
${}^2_5I_{5\frac{1}{2}}$	${}^2_5F_{3\frac{1}{2}}$	$-(2730)^{1/2}/39$	0	${}^2_3H_{5\frac{1}{2}}$	${}^2_5F_{3\frac{1}{2}}$	$-5(42)^{1/2}/21$	0
${}^2_5I_{5\frac{1}{2}}$	${}^2_3D_{2\frac{1}{2}}$	$-16(910)^{1/2}/273$	0	${}^2_3H_{5\frac{1}{2}}$	${}^2_1D_{2\frac{1}{2}}$	$-8(10)^{1/2}/3$	0
${}^2_5I_{6\frac{1}{2}}$	${}^2_3H_{5\frac{1}{2}}$	$-20(546)^{1/2}/273$	0	${}^2_3H_{5\frac{1}{2}}$	${}^2_5D_{2\frac{1}{2}}$	$-16(35)^{1/2}/21$	0
${}^2_4I_{6\frac{1}{2}}$	${}^2_3G_{3\frac{1}{2}}$	$-10(39)^{1/2}/91$	0	${}^2_3G_{3\frac{1}{2}}$	${}^2_5G_{3\frac{1}{2}}$	$39(165)^{1/2}/77$	$(165)^{1/2}/12$
${}^2_5I_{6\frac{1}{2}}$	${}^2_3F_{2\frac{1}{2}}$	$-16(195)^{1/2}/273$	0	${}^2_3G_{3\frac{1}{2}}$	${}^2_5F_{2\frac{1}{2}}$	$-30/7$	0
${}^2_5I_{6\frac{1}{2}}$	${}^2_3F_{3\frac{1}{2}}$	$90(65)^{1/2}/91$	0	${}^2_3G_{3\frac{1}{2}}$	${}^2_5F_{3\frac{1}{2}}$	$-15(3)^{1/2}/7$	$-3(3)^{1/2}/4$
${}^2_5I_{6\frac{1}{2}}$	${}^2_3D_{2\frac{1}{2}}$	$-32(195)^{1/2}/273$	0	${}^2_3G_{3\frac{1}{2}}$	${}^2_1D_{2\frac{1}{2}}$	$-4(35)^{1/2}/7$	0
${}^2_5I_{6\frac{1}{2}}$	${}^2_3H_{5\frac{1}{2}}$	$-5(385)^{1/2}/66$	0	${}^2_3G_{3\frac{1}{2}}$	${}^2_5D_{2\frac{1}{2}}$	$(10)^{1/2}/7$	0
${}^2_5I_{6\frac{1}{2}}$	${}^2_3G_{3\frac{1}{2}}$	$5(110)^{1/2}/462$	0	${}^2_5G_{3\frac{1}{2}}$	${}^2_3F_{2\frac{1}{2}}$	$-10(33)^{1/2}/11$	0
${}^2_5I_{6\frac{1}{2}}$	${}^2_3F_{2\frac{1}{2}}$	$85(22)^{1/2}/924$	0	${}^2_5G_{3\frac{1}{2}}$	${}^2_3F_{3\frac{1}{2}}$	$-15(11)^{1/2}/11$	$(11)^{1/2}/4$
${}^2_5G_{3\frac{1}{2}}$	${}^2_3D_{2\frac{1}{2}}$	$-30(33)^{1/2}/77$	0				
${}^2_5F_{2\frac{1}{2}}$	${}^2_5F_{2\frac{1}{2}}$	$22(5)^{1/2}/21$	$(5)^{1/2}/3$				
${}^2_3F_{2\frac{1}{2}}$	${}^2_5F_{3\frac{1}{2}}$	$-10(15)^{1/2}/21$	0				
${}^2_3F_{2\frac{1}{2}}$	${}^2_1D_{2\frac{1}{2}}$	$40(7)^{1/2}/21$	$-2(7)^{1/2}/3$				
${}^2_3F_{2\frac{1}{2}}$	${}^2_5D_{2\frac{1}{2}}$	$10(2)^{1/2}/3$	$-4(2)^{1/2}/3$				
${}^2_3F_{3\frac{1}{2}}$	${}^2_5F_{2\frac{1}{2}}$	$-10(15)^{1/2}/21$	0				
${}^2_3F_{3\frac{1}{2}}$	${}^2_5F_{3\frac{1}{2}}$	$9(5)^{1/2}/7$	$-(5)^{1/2}/4$				
${}^2_3F_{3\frac{1}{2}}$	${}^2_1D_{2\frac{1}{2}}$	$20(21)^{1/2}/21$	0				
${}^2_3F_{3\frac{1}{2}}$	${}^2_5D_{2\frac{1}{2}}$	$5(6)^{1/2}/3$	0				
${}^2_5F_{2\frac{1}{2}}$	${}^2_2D_{2\frac{1}{2}}$	$44(5)^{1/2}/21$	$2(5)^{1/2}/3$				
${}^2_5F_{3\frac{1}{2}}$	${}^2_5D_{2\frac{1}{2}}$	$22(15)^{1/2}/21$	0				
${}^2_1D_{2\frac{1}{2}}$	${}^2_3D_{2\frac{1}{2}}$	$20(7)^{1/2}/21$	$-(7)^{1/2}/3$				
${}^2_3D_{2\frac{1}{2}}$	${}^2_5D_{2\frac{1}{2}}$	$-40(2)^{1/2}/21$	$(2)^{1/2}/3$				

Table 3. Non-vanishing matrix elements of $(d^5v'S'L'J'\Gamma_8|V_{oct} + V_{so}|d^5vSLJ\Gamma_8)$

$v'S'L'J'$	$vSLJ$	Dq	ζ_{nd}	$v'S'L'J'$	$vSLJ$	Dq	ζ_{nd}
${}^6_5S_{2\frac{1}{2}}$	${}^4_3P_{2\frac{1}{2}}$	0	$-(5)^{1/2}$	${}^4_5G_{3\frac{1}{2}}$	${}^4_3P_{2\frac{1}{2}}$	$-6(10)^{1/2}/5$	0
${}^4_5G_{2\frac{1}{2}}$	${}^4_3F_{1\frac{1}{2}}$	$11(70)^{1/2}/49$	0	${}^4_5G_{3\frac{1}{2}}$	${}^2_3G_{3\frac{1}{2}}$	0	$-(42)^{1/2}/12$
${}^4_5G_{2\frac{1}{2}}$	${}^4_3F_{2\frac{1}{2}}$	$11(105)^{1/2}/49$	$(105)^{1/2}/14$	${}^4_5G_{3\frac{1}{2}}$	${}^2_3F_{3\frac{1}{2}}$	0	$-5(70)^{1/2}/28$
${}^4_5G_{2\frac{1}{2}}$	${}^4_3F_{3\frac{1}{2}}$	$20(35)^{1/2}/49$	0	${}^4_5G_{4\frac{1}{2}}$	${}^4_3F_{1\frac{1}{2}}$	$-3(231)^{1/2}/77$	0
${}^4_5G_{2\frac{1}{2}}$	${}^4_3F_{4\frac{1}{2}}$	$-5(10)^{1/2}/14$	0	${}^4_5G_{4\frac{1}{2}}$	${}^4_3F_{2\frac{1}{2}}$	$51(154)^{1/2}/154$	0
${}^4_5G_{2\frac{1}{2}}$	${}^4_3F_{4\frac{1}{2}}$	$-5(210)^{1/2}/294$	0	${}^4_5G_{4\frac{1}{2}}$	${}^4_3F_{3\frac{1}{2}}$	$-20(462)^{1/2}/693$	0
${}^4_5G_{2\frac{1}{2}}$	${}^4_3P_{1\frac{1}{2}}$	$(30)^{1/2}$	0	${}^4_5G_{4\frac{1}{2}}$	${}^4_3F_{4\frac{1}{2}}$	$-85(33)^{1/2}/198$	$(33)^{1/2}/6$
${}^4_5G_{2\frac{1}{2}}$	${}^4_3P_{2\frac{1}{2}}$	$(30)^{1/2}/3$	0	${}^4_5G_{4\frac{1}{2}}$	${}^4_3F_{4\frac{1}{2}}$	$125(77)^{1/2}/462$	$(33)^{1/2}/6$
${}^4_5G_{2\frac{1}{2}}$	${}^2_3F_{2\frac{1}{2}}$	0	$-5(42)^{1/2}/14$	${}^4_5G_{4\frac{1}{2}}$	${}^4_3P_{1\frac{1}{2}}$	$(11)^{1/2}/33$	0
${}^4_5G_{3\frac{1}{2}}$	${}^4_3F_{1\frac{1}{2}}$	$-66(210)^{1/2}/245$	0	${}^4_5G_{4\frac{1}{2}}$	${}^4_3P_{2\frac{1}{2}}$	$-21(11)^{1/2}/11$	0
${}^4_5G_{3\frac{1}{2}}$	${}^4_3F_{2\frac{1}{2}}$	$12(35)^{1/2}/245$	0	${}^4_5G_{4\frac{1}{2}}$	${}^4_3H_{4\frac{1}{2}}$	0	$2(5)^{1/2}/5$
${}^4_5G_{3\frac{1}{2}}$	${}^4_3F_{3\frac{1}{2}}$	$22(105)^{1/2}/441$	$2(105)^{1/2}/21$	${}^4_5G_{4\frac{1}{2}}$	${}^4_3H_{4\frac{1}{2}}$	0	$2(5)^{1/2}/5$
${}^4_5G_{3\frac{1}{2}}$	${}^4_3F_{4\frac{1}{2}}$	$20(30)^{1/2}/63$	0	${}^4_5G_{4\frac{1}{2}}$	${}^2_3G_{4\frac{1}{2}}$	0	$-(330)^{1/2}/30$
${}^4_5G_{3\frac{1}{2}}$	${}^4_3F_{4\frac{1}{2}}$	$-40(70)^{1/2}/147$	0	${}^4_5G_{4\frac{1}{2}}$	${}^2_3G_{4\frac{1}{2}}$	0	$-(330)^{1/2}/30$
${}^4_5G_{3\frac{1}{2}}$	${}^4_3P_{1\frac{1}{2}}$	$16(10)^{1/2}/15$	0	${}^4_5G_{4\frac{1}{2}}$	${}^4_3F_{1\frac{1}{2}}$	$-9(11)^{1/2}/11$	0
${}^4_5G_{4\frac{1}{2}}$	${}^4_3F_{2\frac{1}{2}}$	$17(66)^{1/2}/154$	0	${}^4_5G_{5\frac{1}{2}}$	${}^4_3P_{1\frac{1}{2}}$	$8(165)^{1/2}/55$	0
${}^4_5G_{4\frac{1}{2}}$	${}^4_3F_{3\frac{1}{2}}$	$40(22)^{1/2}/231$	0	${}^4_5G_{5\frac{1}{2}}$	${}^4_3P_{2\frac{1}{2}}$	$-52(165)^{1/2}/165$	0
${}^4_5G_{4\frac{1}{2}}$	${}^4_3F_{4\frac{1}{2}}$	$125(77)^{1/2}/462$	$(33)^{1/2}/6$	${}^4_5G_{5\frac{1}{2}}$	${}^2_3H_{5\frac{1}{2}}$	0	$(3)^{1/2}$
${}^4_5G_{4\frac{1}{2}}$	${}^4_3F_{4\frac{1}{2}}$	$5(33)^{1/2}/66$	$(33)^{1/2}/6$	${}^4_5G_{5\frac{1}{2}}$	${}^2_3H_{5\frac{1}{2}}$	0	$(3)^{1/2}$
${}^4_5G_{4\frac{1}{2}}$	${}^4_3P_{1\frac{1}{2}}$	$(231)^{1/2}/33$	0	${}^4_5G_{5\frac{1}{2}}$	${}^4_3F_{1\frac{1}{2}}$	$-4(154)^{1/2}/77$	0
${}^4_5G_{4\frac{1}{2}}$	${}^4_3P_{2\frac{1}{2}}$	$-(231)^{1/2}/11$	0	${}^4_5G_{5\frac{1}{2}}$	${}^4_3F_{2\frac{1}{2}}$	$-4(231)^{1/2}/77$	0
${}^4_5G_{4\frac{1}{2}}$	${}^2_3H_{4\frac{1}{2}}$	0	$2(5)^{1/2}/5$	${}^4_5G_{5\frac{1}{2}}$	${}^4_3F_{3\frac{1}{2}}$	$-20(77)^{1/2}/77$	0
${}^4_5G_{4\frac{1}{2}}$	${}^4_3H_{4\frac{1}{2}}$	0	$2(5)^{1/2}/5$	${}^4_5G_{5\frac{1}{2}}$	${}^4_3F_{4\frac{1}{2}}$	$20(462)^{1/2}/231$	0

Table 3 (cont.)

$v'S'L'J'$	$vSLJ$	Dq	ζ_{nd}	$v'S'L'J'$	$vSLJ$	Dq	ζ_{nd}
${}^4_5G_{4\frac{1}{2}}'$	${}^4_3G_{4\frac{1}{2}}$	0	$-(330)^{1/2}/30$	${}^4_5G_{6\frac{1}{2}}'$	${}^4_3F_{1\frac{1}{2}}$	$-8(66)^{1/2}/11$	0
${}^4_5G_{4\frac{1}{2}}'$	${}^4_3G_{4\frac{1}{2}}'$	0	$-(330)^{1/2}/30$	${}^4_5G_{5\frac{1}{2}}'$	${}^4_3P_{2\frac{1}{2}}$	$-8(66)^{1/2}/33$	0
${}^4_5G_{5\frac{1}{2}}$	${}^4_3F_{1\frac{1}{2}}$	$4(385)^{1/2}/385$	0	${}^4_5G_{5\frac{1}{2}}'$	${}^4_3H_{5\frac{1}{2}}$	0	$(3)^{1/2}$
${}^4_5G_{5\frac{1}{2}}$	${}^4_3F_{3\frac{1}{2}}$	$-13(2310)^{1/2}/385$	0	${}^4_5G_{5\frac{1}{2}}$	${}^4_3H_{5\frac{1}{2}}'$	0	$(3)^{1/2}$
${}^4_5G_{5\frac{1}{2}}$	${}^4_3F_{3\frac{1}{2}}$	$-6(770)^{1/2}/77$	0	${}^4_3F_{1\frac{1}{2}}$	${}^4_5D_{1\frac{1}{2}}$	0	$2(5)^{1/2}/5$
${}^4_5G_{5\frac{1}{2}}$	${}^4_3F_{4\frac{1}{2}}$	$-5(55)^{1/2}/11$	0	${}^4_3F_{1\frac{1}{2}}$	${}^4_5D_{2\frac{1}{2}}$	$20(105)^{1/2}/49$	0
${}^4_5G_{5\frac{1}{2}}$	${}^4_3F_{4\frac{1}{2}}'$	$-25(1155)^{1/2}/231$	0	${}^4_3F_{1\frac{1}{2}}$	${}^4_5D_{3\frac{1}{2}}$	$-60(42)^{1/2}/147$	0
${}^4_3F_{1\frac{1}{2}}$	${}^2_2D_{1\frac{1}{2}}$	0	$(70)^{1/2}/5$	${}^4_3F_{4\frac{1}{2}}$	${}^4_5D_{3\frac{1}{2}}$	$20(6)^{1/2}/21$	0
${}^4_3F_{1\frac{1}{2}}$	${}^2_2D_{1\frac{1}{2}}$	0	$(5)^{1/2}/5$	${}^4_3F_{4\frac{1}{2}}$	${}^2_2G_{4\frac{1}{2}}$	0	$(66)^{1/2}/6$
${}^4_3F_{3\frac{1}{2}}$	${}^4_5D_{1\frac{1}{2}}$	$5(30)^{1/2}/7$	0	${}^4_3F_{4\frac{1}{2}}$	${}^2_2G_{4\frac{1}{2}}'$	0	$(66)^{1/2}/6$
${}^4_3F_{2\frac{1}{2}}$	${}^4_5D_{2\frac{1}{2}}$	$-5(70)^{1/2}/49$	$16(70)^{1/2}/105$	${}^4_3F_{4\frac{1}{2}}'$	${}^4_5D_{1\frac{1}{2}}$	$(15)^{1/2}$	0
${}^4_3F_{2\frac{1}{2}}$	${}^4_5D_{2\frac{1}{2}}$	$-60(7)^{1/2}/49$	0	${}^4_3F_{4\frac{1}{2}}'$	${}^4_5D_{2\frac{1}{2}}$	$-9(35)^{1/2}$	0
${}^4_3F_{2\frac{1}{2}}$	${}^2_2F_{2\frac{1}{2}}$	0	$-5(2)^{1/2}/6$	${}^4_3F_{4\frac{1}{2}}'$	${}^4_5D_{3\frac{1}{2}}$	$-40(14)^{1/2}/49$	0
${}^4_3F_{2\frac{1}{2}}$	${}^2_2D_{3\frac{1}{2}}$	0	$2(70)^{1/2}/15$	${}^4_3F_{4\frac{1}{2}}'$	${}^2_2G_{4\frac{1}{2}}$	0	$(66)^{1/2}/6$
${}^4_3F_{2\frac{1}{2}}$	${}^2_2D_{2\frac{1}{2}}$	0	$2(5)^{1/2}/15$	${}^4_3F_{4\frac{1}{2}}'$	${}^2_2G_{4\frac{1}{2}}'$	0	$(66)^{1/2}/6$
${}^4_3F_{3\frac{1}{2}}$	${}^4_5D_{1\frac{1}{2}}$	$4(10)^{1/2}/7$	0	${}^4_5D_{1\frac{1}{2}}$	${}^4_3P_{1\frac{1}{2}}$	0	$2(105)^{1/2}/15$
${}^4_3F_{3\frac{1}{2}}$	${}^4_5D_{2\frac{1}{2}}$	$-6(210)^{1/2}/49$	0	${}^4_5D_{1\frac{1}{2}}$	${}^3_3D_{1\frac{1}{2}}$	0	$-(2)^{1/2}$
${}^4_3F_{3\frac{1}{2}}$	${}^4_5D_{3\frac{1}{2}}$	$-20(21)^{1/2}/147$	$2(21)^{1/2}/7$	${}^4_5D_{1\frac{1}{2}}$	${}^3_3P_{1\frac{1}{2}}$	0	$-(3)^{1/2}/3$
${}^4_3F_{3\frac{1}{2}}$	${}^2_2G_{3\frac{1}{2}}$	0	$(66)^{1/2}/12$	${}^4_5D_{2\frac{1}{2}}$	${}^4_3P_{2\frac{1}{2}}$	0	$7(5)^{1/2}/10$
${}^4_3F_{3\frac{1}{2}}$	${}^2_2F_{3\frac{1}{2}}$	0	$-(30)^{1/2}/4$	${}^4_5D_{2\frac{1}{2}}$	${}^3_3F_{2\frac{1}{2}}$	0	$-4(7)^{1/2}/21$
${}^4_3F_{4\frac{1}{2}}$	${}^4_5D_{1\frac{1}{2}}$	$(35)^{1/2}/7$	0	${}^4_5D_{2\frac{1}{2}}$	${}^3_3D_{2\frac{1}{2}}$	0	$-2(7)^{1/2}/3$
${}^4_3F_{4\frac{1}{2}}$	${}^4_5D_{2\frac{1}{2}}$	$-9(15)^{1/2}/7$	0	${}^3_3D_{3\frac{1}{2}}$	${}^3_3F_{3\frac{1}{2}}$	0	$-2(14)^{1/2}/7$
${}^2_2P_{1\frac{1}{2}}$	${}^2_2D_{1\frac{1}{2}}$	0	$2(30)^{1/2}/15$	${}^2_2I_{5\frac{1}{2}}'$	${}^2_3H_{4\frac{1}{2}}'$	$-32(2730)^{1/2}/429$	0
${}^2_2P_{1\frac{1}{2}}$	${}^2_2D_{1\frac{1}{2}}$	0	$(105)^{1/2}/15$	${}^2_2I_{5\frac{1}{2}}'$	${}^2_3H_{5\frac{1}{2}}$	$20(130)^{1/2}/429$	$(13)^{1/2}/2$
${}^2_2P_{2\frac{1}{2}}$	${}^2_2D_{2\frac{1}{2}}$	0	$4(5)^{1/2}/5$	${}^2_2I_{5\frac{1}{2}}'$	${}^2_3H_{5\frac{1}{2}}'$	$-380(13)^{1/2}/429$	$(13)^{1/2}/2$
${}^2_2P_{2\frac{1}{2}}$	${}^2_2D_{2\frac{1}{2}}$	0	$(70)^{1/2}/5$	${}^2_2I_{5\frac{1}{2}}'$	${}^2_3G_{3\frac{1}{2}}$	$-5(30030)^{1/2}/1001$	0
${}^2_2I_{5\frac{1}{2}}$	${}^2_3H_{4\frac{1}{2}}$	$280(13)^{1/2}/143$	0	${}^2_2I_{5\frac{1}{2}}'$	${}^2_3G_{4\frac{1}{2}}$	$-4(5005)^{1/2}/1001$	0
${}^2_2I_{5\frac{1}{2}}$	${}^2_3H_{4\frac{1}{2}}'$	$200(273)^{1/2}/429$	0	${}^2_2I_{5\frac{1}{2}}'$	${}^2_3F_{2\frac{1}{2}}$	$10(10010)^{1/2}/429$	0
${}^2_2I_{5\frac{1}{2}}$	${}^2_3H_{5\frac{1}{2}}$	$280(13)^{1/2}/429$	$(13)^{1/2}/2$	${}^2_2I_{5\frac{1}{2}}'$	${}^2_3F_{3\frac{1}{2}}$	$-5(2002)^{1/2}/143$	0
${}^2_2I_{5\frac{1}{2}}$	${}^2_3H_{5\frac{1}{2}}'$	$20(130)^{1/2}/429$	$(13)^{1/2}/2$	${}^2_2I_{5\frac{1}{2}}'$	${}^3_3D_{1\frac{1}{2}}$	$8(15015)^{1/2}/231$	0
${}^2_2I_{5\frac{1}{2}}$	${}^2_3G_{3\frac{1}{2}}$	$-15(3003)^{1/2}/1001$	0	${}^2_2I_{5\frac{1}{2}}'$	${}^3_3D_{2\frac{1}{2}}$	$-16(10010)^{1/2}/3003$	0
${}^2_2I_{5\frac{1}{2}}$	${}^2_3G_{4\frac{1}{2}}$	$5(858)^{1/2}/286$	0	${}^2_2I_{6\frac{1}{2}}$	${}^2_3H_{4\frac{1}{2}}$	$2(78)^{1/2}/143$	0
${}^2_2I_{5\frac{1}{2}}$	${}^2_3G_{4\frac{1}{2}}'$	$25(2002)^{1/2}/2002$	0	${}^2_2I_{6\frac{1}{2}}$	${}^2_3H_{4\frac{1}{2}}'$	$-30(182)^{1/2}/143$	0
${}^2_2I_{5\frac{1}{2}}$	${}^2_3F_{2\frac{1}{2}}$	$5(1001)^{1/2}/33$	0	${}^2_2I_{6\frac{1}{2}}$	${}^2_3H_{5\frac{1}{2}}$	$-152(78)^{1/2}/429$	0
${}^2_2I_{5\frac{1}{2}}$	${}^2_3F_{1\frac{1}{2}}$	$-3(5005)^{1/2}/143$	0	${}^2_2I_{6\frac{1}{2}}$	${}^2_3H_{5\frac{1}{2}}'$	$-248(195)^{1/2}/429$	0
${}^2_2I_{5\frac{1}{2}}$	${}^2_3D_{1\frac{1}{2}}$	$-4(6006)^{1/2}/231$	0	${}^2_2I_{6\frac{1}{2}}$	${}^2_3H_{5\frac{1}{2}}'$	$-31(2002)^{1/2}/3003$	0
${}^2_2I_{5\frac{1}{2}}$	${}^2_3D_{2\frac{1}{2}}$	$-8(1001)^{1/2}/231$	0	${}^2_2I_{6\frac{1}{2}}$	${}^2_3G_{3\frac{1}{2}}$	$-2(143)^{1/2}/429$	0
${}^2_2I_{6\frac{1}{2}}$	${}^2_3G_{4\frac{1}{2}}'$	$70(3003)^{1/2}/3003$	0	${}^2_3H_{4\frac{1}{2}}$	${}^2_2F_{2\frac{1}{2}}$	$13(385)^{1/2}/77$	0
${}^2_2I_{6\frac{1}{2}}$	${}^2_3F_{2\frac{1}{2}}$	$20(6006)^{1/2}/3003$	0	${}^2_3H_{4\frac{1}{2}}$	${}^2_2F_{3\frac{1}{2}}$	$10(77)^{1/2}/77$	0
${}^2_2I_{6\frac{1}{2}}$	${}^2_3F_{3\frac{1}{2}}$	$31(30030)^{1/2}/1001$	0	${}^2_3H_{4\frac{1}{2}}$	${}^2_1D_{1\frac{1}{2}}$	$-2(66)^{1/2}/11$	0
${}^2_2I_{6\frac{1}{2}}$	${}^2_3D_{2\frac{1}{2}}$	$40(6006)^{1/2}/3003$	0	${}^2_3H_{4\frac{1}{2}}$	${}^2_1D_{2\frac{1}{2}}$	$-14(11)^{1/2}/11$	0
${}^2_2I_{6\frac{1}{2}}'$	${}^2_3H_{4\frac{1}{2}}$	$24(143)^{1/2}/143$	0	${}^2_3H_{4\frac{1}{2}}$	${}^2_2D_{1\frac{1}{2}}$	$-4(231)^{1/2}/77$	0
${}^2_2I_{6\frac{1}{2}}'$	${}^2_3H_{5\frac{1}{2}}$	$32(143)^{1/2}/143$	0	${}^2_3H_{4\frac{1}{2}}$	${}^2_2D_{2\frac{1}{2}}$	$-2(154)^{1/2}/11$	0
${}^2_2I_{6\frac{1}{2}}'$	${}^2_3H_{5\frac{1}{2}}'$	$4(1430)^{1/2}/143$	0	${}^2_3H_{4\frac{1}{2}}'$	${}^2_2G_{3\frac{1}{2}}$	$-20(15)^{1/2}/33$	0
${}^2_2I_{6\frac{1}{2}}'$	${}^2_3G_{4\frac{1}{2}}$	$-4(273)^{1/2}/273$	0	${}^2_3H_{4\frac{1}{2}}'$	${}^2_2G_{4\frac{1}{2}}$	$-25(210)^{1/2}/462$	$2(10)^{1/2}/5$
${}^2_2I_{6\frac{1}{2}}'$	${}^2_3G_{4\frac{1}{2}}'$	$-4(78)^{1/2}/39$	0	${}^2_3H_{4\frac{1}{2}}'$	${}^2_2G_{4\frac{1}{2}}'$	$-(10)^{1/2}/22$	$2(10)^{1/2}/5$
${}^2_2I_{6\frac{1}{2}}'$	${}^2_3F_{2\frac{1}{2}}$	$-20(91)^{1/2}/91$	0	${}^2_3H_{4\frac{1}{2}}'$	${}^2_2F_{2\frac{1}{2}}$	$13(165)^{1/2}/231$	0
${}^2_2I_{6\frac{1}{2}}'$	${}^2_3F_{3\frac{1}{2}}$	$12(455)^{1/2}/91$	0	${}^2_3H_{4\frac{1}{2}}'$	${}^2_2F_{1\frac{1}{2}}$	$-20(33)^{1/2}/77$	0
${}^2_2I_{6\frac{1}{2}}'$	${}^2_3D_{2\frac{1}{2}}$	$-40(91)^{1/2}/91$	0	${}^2_3H_{4\frac{1}{2}}'$	${}^2_1D_{1\frac{1}{2}}$	$-6(154)^{1/2}/11$	0
${}^2_3H_{4\frac{1}{2}}$	${}^2_2G_{3\frac{1}{2}}$	$10(35)^{1/2}/33$	0	${}^2_3H_{4\frac{1}{2}}'$	${}^2_1D_{2\frac{1}{2}}$	$-2(231)^{1/2}/33$	0
${}^2_3H_{4\frac{1}{2}}$	${}^2_2G_{4\frac{1}{2}}$	$17(10)^{1/2}/66$	$2(10)^{1/2}/5$	${}^2_3H_{4\frac{1}{2}}'$	${}^2_2D_{1\frac{1}{2}}$	$-12(11)^{1/2}/11$	0

Table 3 (cont.)

$v'S'L'J'$	$vSLJ$	Dq	ζ_{nd}	$v'S'L'J'$	$vSLJ$	Dq	ζ_{nd}
${}^2_3H_{4\frac{1}{2}}$	${}^2_5G_{4\frac{1}{2}}$	$-25(210)^{1/2}/462$	$2(10)^{1/2}/5$	${}^2_3H_{4\frac{1}{2}}$	${}^2_5D_{2\frac{1}{2}}$	$-2(66)^{1/2}/33$	0
${}^2_3H_{5\frac{1}{2}}$	${}^2_5G_{3\frac{1}{2}}$	$9(35)^{1/2}/77$	0	${}^2_3H_{5\frac{1}{2}}$	${}^2_5D_{1\frac{1}{2}}$	$-8(2310)^{1/2}/231$	0
${}^2_3H_{5\frac{1}{2}}$	${}^2_5G_{4\frac{1}{2}}$	$15(10)^{1/2}/22$	0	${}^2_3H_{5\frac{1}{2}}$	${}^2_5D_{2\frac{1}{2}}$	$-16(385)^{1/2}/231$	0
${}^2_3H_{5\frac{1}{2}}$	${}^2_5G_{4\frac{1}{2}}$	$25(210)^{1/2}/154$	0	${}^2_3G_{3\frac{1}{2}}$	${}^2_5G_{3\frac{1}{2}}$	$-13(165)^{1/2}/231$	$(165)^{1/2}/12$
${}^2_3H_{5\frac{1}{2}}$	${}^2_5F_{2\frac{1}{2}}$	$-13(385)^{1/2}/231$	0	${}^2_3G_{3\frac{1}{2}}$	${}^2_5G_{4\frac{1}{2}}$	$-10(2310)^{1/2}/231$	0
${}^2_3H_{5\frac{1}{2}}$	${}^2_5F_{3\frac{1}{2}}$	$-15(77)^{1/2}/77$	0	${}^2_3G_{3\frac{1}{2}}$	${}^2_5G_{4\frac{1}{2}}$	$20(11)^{1/2}/77$	0
${}^2_3H_{5\frac{1}{2}}$	${}^2_1D_{1\frac{1}{2}}$	$4(66)^{1/2}/33$	0	${}^2_3G_{3\frac{1}{2}}$	${}^2_5F_{2\frac{1}{2}}$	$-6(15)^{1/2}/7$	0
${}^2_3H_{5\frac{1}{2}}$	${}^2_1D_{2\frac{1}{2}}$	$-52(11)^{1/2}/33$	0	${}^2_3G_{3\frac{1}{2}}$	${}^2_5F_{3\frac{1}{2}}$	$5(3)^{1/2}/21$	$-3(3)^{1/2}/4$
${}^2_3H_{5\frac{1}{2}}$	${}^2_5D_{1\frac{1}{2}}$	$8(231)^{1/2}/231$	0	${}^2_3G_{3\frac{1}{2}}$	${}^2_1D_{1\frac{1}{2}}$	$22(14)^{1/2}/21$	0
${}^2_3H_{5\frac{1}{2}}$	${}^2_5D_{2\frac{1}{2}}$	$-52(154)^{1/2}/231$	0	${}^2_3G_{3\frac{1}{2}}$	${}^2_1D_{2\frac{1}{2}}$	$-4(21)^{1/2}/7$	0
${}^2_3H_{5\frac{1}{2}}$	${}^2_5G_{3\frac{1}{2}}$	$15(14)^{1/2}/77$	0	${}^2_3G_{3\frac{1}{2}}$	${}^2_2D_{1\frac{1}{2}}$	$-11/21$	0
${}^2_3H_{5\frac{1}{2}}$	${}^2_5G_{4\frac{1}{2}}$	$-20(21)^{1/2}/77$	0	${}^2_3G_{3\frac{1}{2}}$	${}^2_2D_{2\frac{1}{2}}$	$(6)^{1/2}/7$	0
${}^2_3H_{5\frac{1}{2}}$	${}^2_5F_{2\frac{1}{2}}$	$-10(154)^{1/2}/231$	0	${}^2_3G_{4\frac{1}{2}}$	${}^2_5G_{3\frac{1}{2}}$	$-10(2310)^{1/2}/231$	0
${}^2_3H_{5\frac{1}{2}}$	${}^2_5F_{3\frac{1}{2}}$	$-5(770)^{1/2}/77$	0	${}^2_3G_{4\frac{1}{2}}$	${}^2_5G_{4\frac{1}{2}}$	$17(165)^{1/2}/66$	$-(165)^{1/2}/15$
${}^2_3H_{5\frac{1}{2}}$	${}^2_1D_{1\frac{1}{2}}$	$-8(165)^{1/2}/33$	0	${}^2_3G_{4\frac{1}{2}}$	${}^2_5G_{4\frac{1}{2}}$	$-25(385)^{1/2}/154$	$-(165)^{1/2}/15$
${}^2_3H_{5\frac{1}{2}}$	${}^2_1D_{2\frac{1}{2}}$	$-8(110)^{1/2}/33$	0	${}^2_3G_{4\frac{1}{2}}$	${}^2_5F_{2\frac{1}{2}}$	$3(210)^{1/2}/14$	0
${}^2_3G_{4\frac{1}{2}}$	${}^2_5F_{3\frac{1}{2}}$	$-10(42)^{1/2}/21$	0	${}^2_5G_{3\frac{1}{2}}$	${}^2_5F_{3\frac{1}{2}}$	$5(11)^{1/2}/33$	$(11)^{1/2}/4$
${}^2_3G_{4\frac{1}{2}}$	${}^2_1D_{1\frac{1}{2}}$	$2/3$	0	${}^2_5G_{3\frac{1}{2}}$	${}^2_3D_{1\frac{1}{2}}$	$(330)^{1/2}/7$	0
${}^2_3G_{4\frac{1}{2}}$	${}^2_1D_{2\frac{1}{2}}$	$-2(6)^{1/2}$	0	${}^2_5G_{3\frac{1}{2}}$	${}^2_3D_{2\frac{1}{2}}$	$-18(55)^{1/2}/77$	0
${}^2_3G_{4\frac{1}{2}}$	${}^2_5D_{1\frac{1}{2}}$	$-(14)^{1/2}/42$	0	${}^2_5G_{3\frac{1}{2}}$	${}^2_3P_{1\frac{1}{2}}$	$(55)^{1/2}/3$	0
${}^2_3G_{4\frac{1}{2}}$	${}^2_5D_{2\frac{1}{2}}$	$(21)^{1/2}/7$	0	${}^2_5G_{4\frac{1}{2}}$	${}^2_3F_{2\frac{1}{2}}$	$3(770)^{1/2}/22$	0
${}^2_3G_{4\frac{1}{2}}$	${}^2_5G_{3\frac{1}{2}}$	$20(110)^{1/2}/77$	0	${}^2_5G_{4\frac{1}{2}}$	${}^2_3F_{3\frac{1}{2}}$	$-10(154)^{1/2}/33$	0
${}^2_3G_{4\frac{1}{2}}$	${}^2_5G_{4\frac{1}{2}}$	$-25(385)^{1/2}/154$	$-(165)^{1/2}/15$	${}^2_5G_{4\frac{1}{2}}$	${}^2_3D_{1\frac{1}{2}}$	$(1155)^{1/2}/77$	0
${}^2_3G_{4\frac{1}{2}}$	${}^2_5G_{4\frac{1}{2}}$	$-(165)^{1/2}/22$	$-(165)^{1/2}/15$	${}^2_5G_{4\frac{1}{2}}$	${}^2_3D_{2\frac{1}{2}}$	$-9(770)^{1/2}/77$	0
${}^2_3G_{4\frac{1}{2}}$	${}^2_5F_{2\frac{1}{2}}$	$3(10)^{1/2}/14$	0	${}^2_5G_{4\frac{1}{2}}$	${}^2_3P_{1\frac{1}{2}}$	$-(770)^{1/2}/42$	0
${}^2_3G_{4\frac{1}{2}}$	${}^2_5F_{3\frac{1}{2}}$	$20(2)^{1/2}/7$	0	${}^2_5G_{4\frac{1}{2}}$	${}^2_3F_{2\frac{1}{2}}$	$(330)^{1/2}/22$	0
${}^2_3G_{4\frac{1}{2}}$	${}^2_1D_{1\frac{1}{2}}$	$2(21)^{1/2}/3$	0	${}^2_5G_{4\frac{1}{2}}$	${}^2_3F_{1\frac{1}{2}}$	$20(66)^{1/2}/33$	0
${}^2_3G_{4\frac{1}{2}}$	${}^2_1D_{2\frac{1}{2}}$	$-2(14)^{1/2}/7$	0	${}^2_5G_{4\frac{1}{2}}$	${}^2_3D_{1\frac{1}{2}}$	$-3(55)^{1/2}/11$	0
${}^2_3G_{4\frac{1}{2}}$	${}^2_5D_{1\frac{1}{2}}$	$-(6)^{1/2}/6$	0	${}^2_5G_{4\frac{1}{2}}$	${}^2_3D_{2\frac{1}{2}}$	$-3(330)^{1/2}/77$	0
${}^2_3G_{4\frac{1}{2}}$	${}^2_5D_{2\frac{1}{2}}$	$1/7$	0	${}^2_5G_{4\frac{1}{2}}$	${}^2_3P_{1\frac{1}{2}}$	$-(330)^{1/2}/6$	0
${}^2_5G_{3\frac{1}{2}}$	${}^2_3F_{2\frac{1}{2}}$	$-6(55)^{1/2}/11$	0	${}^2_5F_{2\frac{1}{2}}$	${}^2_5F_{2\frac{1}{2}}$	$-11(5)^{1/2}/21$	$(5)^{1/2}/3$
${}^2_3F_{2\frac{1}{2}}$	${}^2_1F_{1\frac{1}{2}}$	$-10/7$	0	${}^2_5F_{3\frac{1}{2}}$	${}^2_3D_{1\frac{1}{2}}$	$11(6)^{1/2}/7$	0
${}^2_3F_{2\frac{1}{2}}$	${}^2_1D_{1\frac{1}{2}}$	$-10(42)^{1/2}/21$	0	${}^2_5F_{3\frac{1}{2}}$	${}^2_3D_{2\frac{1}{2}}$	$22/7$	0
${}^2_3F_{2\frac{1}{2}}$	${}^2_1D_{2\frac{1}{2}}$	$-20(7)^{1/2}/3$	$-2(7)^{1/2}/3$	${}^2_5F_{3\frac{1}{2}}$	${}^2_3P_{1\frac{1}{2}}$	$15/7$	0
${}^2_3F_{2\frac{1}{2}}$	${}^2_5D_{1\frac{1}{2}}$	$-5(3)^{1/2}/3$	0	${}^2_1D_{1\frac{1}{2}}$	${}^2_3D_{1\frac{1}{2}}$	0	$(7)^{1/2}/2$
${}^2_3F_{2\frac{1}{2}}$	${}^2_5D_{2\frac{1}{2}}$	$-5(2)^{1/2}/3$	$-4(2)^{1/2}/3$	${}^2_1D_{1\frac{1}{2}}$	${}^2_3D_{2\frac{1}{2}}$	$10(42)^{1/2}/21$	0
${}^2_3F_{3\frac{1}{2}}$	${}^2_5F_{2\frac{1}{2}}$	$-10/7$	0	${}^2_1D_{2\frac{1}{2}}$	${}^2_3P_{1\frac{1}{2}}$	0	$(42)^{1/2}/6$
${}^2_3F_{3\frac{1}{2}}$	${}^2_5F_{3\frac{1}{2}}$	$-(5)^{1/2}/7$	$-(5)^{1/2}/4$	${}^2_1D_{2\frac{1}{2}}$	${}^2_3D_{1\frac{1}{2}}$	$10(42)^{1/2}/21$	0
${}^2_3F_{3\frac{1}{2}}$	${}^2_1D_{1\frac{1}{2}}$	$2(210)^{1/2}/7$	0	${}^2_1D_{2\frac{1}{2}}$	${}^2_3D_{2\frac{1}{2}}$	$-10(7)^{1/2}/21$	$-(7)^{1/2}/3$
${}^2_3F_{3\frac{1}{2}}$	${}^2_1D_{2\frac{1}{2}}$	$4(35)^{1/2}/7$	0	${}^2_5D_{1\frac{1}{2}}$	${}^2_5D_{1\frac{1}{2}}$	0	$-(2)^{1/2}/2$
${}^2_3F_{3\frac{1}{2}}$	${}^2_5D_{1\frac{1}{2}}$	$(15)^{1/2}$	0	${}^2_5D_{1\frac{1}{2}}$	${}^2_5D_{2\frac{1}{2}}$	$-40(3)^{1/2}/21$	0
${}^2_3F_{3\frac{1}{2}}$	${}^2_5D_{2\frac{1}{2}}$	$(10)^{1/2}$	0	${}^2_5D_{2\frac{1}{2}}$	${}^2_5D_{1\frac{1}{2}}$	$-40(3)^{1/2}/21$	0
${}^2_3F_{3\frac{1}{2}}$	${}^2_3D_{1\frac{1}{2}}$	$-11(30)^{1/2}/21$	0	${}^2_5D_{2\frac{1}{2}}$	${}^2_5D_{2\frac{1}{2}}$	$20(2)^{1/2}/21$	$(2)^{1/2}/3$
${}^2_3F_{2\frac{1}{2}}$	${}^2_3D_{2\frac{1}{2}}$	$-22(5)^{1/2}/21$	$2(5)^{1/2}/3$	${}^2_5D_{1\frac{1}{2}}$	${}^2_3P_{1\frac{1}{2}}$	0	$-(3)^{1/2}/6$
${}^2_5F_{2\frac{1}{2}}$	${}^2_3P_{1\frac{1}{2}}$	$9(5)^{1/2}/7$	0				

The matrix elements of the weak octahedral field interaction can also be obtained by means of Racah algebra. First the crystal field potential is written in terms of spherical harmonics [7]:

$$V_{oct} = (4/15) D\pi^{1/2} \sum_i r_i^4 [Y_{40}(\theta_i, \varphi_i) + (5/14)^{1/2}(Y_{44}(\theta_i, \varphi_i) + Y_{4-4}(\theta_i, \varphi_i))] \quad (2)$$

Let

$$V_{kp} = \sum Y_{kp}(\theta_i, \varphi_i),$$

then the matrix elements

$$\langle d^n v' S' L' J' M' | V_{kp} | d^n v S L J M \rangle$$

have the following form:

$$\begin{aligned} \langle d^n v' S' L' J' M' | V_{kp} | d^n v S L J M \rangle &= (-1)^{L+k-L'} [(2L+1)(2J'+1)]^{1/2} W(kLJ'S'; L'J) \\ &\times (kJpM | J'M') \langle d^n v' S' L' || V_k || d^n v S L \rangle \quad (3) \end{aligned}$$

For the details of this deviation, see Refs. [3, 4]. The reduced matrix elements $\langle d^n v' S' L' || V_k || d^n v S L \rangle$ in (3) can be calculated by means of a method based on the coefficients of fractional parentage. Explicit formulas are given by BRINK and SATCHLER [8].

As pointed out by FINKELSTEIN and VAN VLECK [9], it is convenient to use as basis functions those which diagonalize the octahedral potential apart from elements non-diagonal in J . Such functions must be classified according to their cubic representation Γ rather than according to their magnetic quantum number M . The transformation matrices $(J\Gamma | JM)$ for $J = 1/2$ to $9/2$ can be found in GRIFFITH'S book. [10] The matrices for $J = 11/2$ and $13/2$ can be calculated by the method outlined in Chapter 6 of the same book. These matrices are reported in the appendix.

The matrix elements $\langle d^5 v' S' L' J' \Gamma_i | V_{oct} + V_{so} | d^5 v S L J \Gamma_i \rangle$, where $i = 6, 7, 8$ and V_{so} is the spin-orbit interaction Hamiltonian, are thereby calculated and the non-vanishing ones are tabulated in Tables 1 to 3. As seen from the Tables, the crystalline field matrix elements are given in terms of the usual parameter Dq , which is also defined in the d^4 paper [4]. These results were checked using other members of degenerate sets.

The primed terms in Tables 2 and 3 arise from the existence of two linearly independent representations having the same classification.

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APPENDIX

Behavior of the *kets* $|JM\rangle$ under the octahedral group for $J = 5\frac{1}{2}$ and $6\frac{1}{2}$. (The notation used here is identical to Griffith's [10].)

$$J = 5\frac{1}{2}$$

$$\begin{aligned} |E'\alpha'\rangle &= (2)^{1/2}/4 |5\frac{1}{2} \frac{1}{2}\rangle - (21)^{1/2}/12 |5\frac{1}{2} 4\frac{1}{2}\rangle - (105)^{1/2}/12 |5\frac{1}{2} - 3\frac{1}{2}\rangle \\ |E'\beta'\rangle &= -(2)^{1/2}/4 |5\frac{1}{2} - \frac{1}{2}\rangle + (21)^{1/2}/12 |5\frac{1}{2} - 4\frac{1}{2}\rangle + (105)^{1/2}/12 |5\frac{1}{2} 3\frac{1}{2}\rangle \\ |E''\alpha''\rangle &= (33)^{1/2}/12 |5\frac{1}{2} 2\frac{1}{2}\rangle + (66)^{1/2}/12 |5\frac{1}{2} - 1\frac{1}{2}\rangle - (5)^{1/2}/4 |5\frac{1}{2} - 5\frac{1}{2}\rangle \\ |E''\beta''\rangle &= -(33)^{1/2}/12 |5\frac{1}{2} - 2\frac{1}{2}\rangle - (66)^{1/2}/12 |5\frac{1}{2} 1\frac{1}{2}\rangle + (5)^{1/2}/4 |5\frac{1}{2} 5\frac{1}{2}\rangle \\ |aU''\kappa\rangle &= -(3)^{1/2}/3 |5\frac{1}{2} 1\frac{1}{2}\rangle + (6)^{1/2}/3 |5\frac{1}{2} - 2\frac{1}{2}\rangle \\ |aU''\lambda\rangle &= -(30)^{1/2}/6 |5\frac{1}{2} 4\frac{1}{2}\rangle + (6)^{1/2}/6 |5\frac{1}{2} - 3\frac{1}{2}\rangle \\ |aU''\mu\rangle &= -(30)^{1/2}/6 |5\frac{1}{2} - 4\frac{1}{2}\rangle + (6)^{1/2}/6 |5\frac{1}{2} 3\frac{1}{2}\rangle \\ |aU''\nu\rangle &= -(3)^{1/2}/3 |5\frac{1}{2} - 1\frac{1}{2}\rangle + (6)^{1/2}/3 |5\frac{1}{2} 2\frac{1}{2}\rangle \\ |bU''\kappa\rangle &= (11)^{1/2}/4 |5\frac{1}{2} 5\frac{1}{2}\rangle + (15)^{1/2}/12 |5\frac{1}{2} - 2\frac{1}{2}\rangle + (30)^{1/2}/12 |5\frac{1}{2} 1\frac{1}{2}\rangle \\ |bU''\lambda\rangle &= (14)^{1/2}/4 |5\frac{1}{2} \frac{1}{2}\rangle + (3)^{1/2}/12 |5\frac{1}{2} 4\frac{1}{2}\rangle + (15)^{1/2}/12 |5\frac{1}{2} - 3\frac{1}{2}\rangle \\ |bU''\mu\rangle &= (14)^{1/2}/4 |5\frac{1}{2} - \frac{1}{2}\rangle + (3)^{1/2}/12 |5\frac{1}{2} - 4\frac{1}{2}\rangle + (15)^{1/2}/12 |5\frac{1}{2} 3\frac{1}{2}\rangle \\ |bU''\nu\rangle &= (11)^{1/2}/4 |5\frac{1}{2} - 5\frac{1}{2}\rangle + (15)^{1/2}/12 |5\frac{1}{2} 2\frac{1}{2}\rangle + (30)^{1/2}/12 |5\frac{1}{2} - 1\frac{1}{2}\rangle \end{aligned}$$

$$J = 6\frac{1}{2}$$

$$\begin{aligned} |E'\alpha'\rangle &= (2)^{1/2}/4 |6\frac{1}{2} \frac{1}{2}\rangle - (11)^{1/2}/4 |6\frac{1}{2} 4\frac{1}{2}\rangle - (3)^{1/2}/4 |6\frac{1}{2} - 3\frac{1}{2}\rangle \\ |E'\beta'\rangle &= (2)^{1/2}/4 |6\frac{1}{2} - \frac{1}{2}\rangle - (11)^{1/2}/4 |6\frac{1}{2} - 4\frac{1}{2}\rangle - (3)^{1/2}/4 |6\frac{1}{2} 3\frac{1}{2}\rangle \\ |aE''\alpha''\rangle &= 3(154)^{1/2}/56 |6\frac{1}{2} 2\frac{1}{2}\rangle + (770)^{1/2}/56 |6\frac{1}{2} - 1\frac{1}{2}\rangle \\ &\quad - (910)^{1/2}/56 |6\frac{1}{2} 6\frac{1}{2}\rangle - (70)^{1/2}/56 |6\frac{1}{2} - 5\frac{1}{2}\rangle \\ |aE''\beta''\rangle &= 3(154)^{1/2}/56 |6\frac{1}{2} - 2\frac{1}{2}\rangle + (770)^{1/2}/56 |6\frac{1}{2} 1\frac{1}{2}\rangle \\ &\quad - (910)^{1/2}/56 |6\frac{1}{2} - 6\frac{1}{2}\rangle - (70)^{1/2}/56 |6\frac{1}{2} 5\frac{1}{2}\rangle \\ |bE''\alpha''\rangle &= (1365)^{1/2}/84 |6\frac{1}{2} 2\frac{1}{2}\rangle - (273)^{1/2}/28 |6\frac{1}{2} - 1\frac{1}{2}\rangle \\ &\quad + (231)^{1/2}/84 |6\frac{1}{2} 6\frac{1}{2}\rangle - (3003)^{1/2}/84 |6\frac{1}{2} - 5\frac{1}{2}\rangle \\ |bE''\beta''\rangle &= (1365)^{1/2}/84 |6\frac{1}{2} - 2\frac{1}{2}\rangle - (273)^{1/2}/28 |6\frac{1}{2} 1\frac{1}{2}\rangle \\ &\quad + (231)^{1/2}/84 |6\frac{1}{2} - 6\frac{1}{2}\rangle - (3003)^{1/2}/84 |6\frac{1}{2} 5\frac{1}{2}\rangle \\ |aU''\kappa\rangle &= (5)^{1/2}/5 |6\frac{1}{2} 1\frac{1}{2}\rangle - \frac{1}{2} |6\frac{1}{2} - 2\frac{1}{2}\rangle - (55)^{1/2}/10 |6\frac{1}{2} 5\frac{1}{2}\rangle \\ |aU''\lambda\rangle &= (110)^{1/2}/20 |6\frac{1}{2} 4\frac{1}{2}\rangle - 3(30)^{1/2}/20 |6\frac{1}{2} - 3\frac{1}{2}\rangle + (5)^{1/2}/10 |6\frac{1}{2} \frac{1}{2}\rangle \\ |aU''\mu\rangle &= -(110)^{1/2}/20 |6\frac{1}{2} - 4\frac{1}{2}\rangle + 3(30)^{1/2}/20 |6\frac{1}{2} 3\frac{1}{2}\rangle - (5)^{1/2}/10 |6\frac{1}{2} - \frac{1}{2}\rangle \\ |aU''\nu\rangle &= -(5)^{1/2}/5 |6\frac{1}{2} - 1\frac{1}{2}\rangle + \frac{1}{2} |6\frac{1}{2} 2\frac{1}{2}\rangle + (55)^{1/2}/10 |6\frac{1}{2} - 5\frac{1}{2}\rangle \\ |bU''\kappa\rangle &= (330)^{1/2}/40 |6\frac{1}{2} 1\frac{1}{2}\rangle + (66)^{1/2}/24 |6\frac{1}{2} - 2\frac{1}{2}\rangle \\ &\quad + (30)^{1/2}/120 |6\frac{1}{2} 5\frac{1}{2}\rangle + (390)^{1/2}/24 |6\frac{1}{2} - 6\frac{1}{2}\rangle \\ |bU''\lambda\rangle &= -(15)^{1/2}/20 |6\frac{1}{2} 4\frac{1}{2}\rangle - (55)^{1/2}/20 |6\frac{1}{2} - 3\frac{1}{2}\rangle - (330)^{1/2}/20 |6\frac{1}{2} \frac{1}{2}\rangle \\ |bU''\mu\rangle &= (15)^{1/2}/20 |6\frac{1}{2} - 4\frac{1}{2}\rangle + (55)^{1/2}/20 |6\frac{1}{2} 3\frac{1}{2}\rangle + (330)^{1/2}/20 |6\frac{1}{2} - \frac{1}{2}\rangle \\ |bU''\nu\rangle &= -(330)^{1/2}/40 |6\frac{1}{2} - 1\frac{1}{2}\rangle - (66)^{1/2}/24 |6\frac{1}{2} 2\frac{1}{2}\rangle \\ &\quad - (30)^{1/2}/120 |6\frac{1}{2} - 5\frac{1}{2}\rangle - (390)^{1/2}/24 |6\frac{1}{2} 6\frac{1}{2}\rangle \end{aligned}$$