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Matrix Elements for Configuration d^4 in a Weak Octahedral Field Using Racah Methods

T. M. DUNN AND WAI-KEE LI
Chemistry Department, University of Michigan, Ann Arbor, Michigan
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Employing Racah algebra, the general formula for calculating the matrix elements of a weak crystalline field for configuration d^n has been derived. Applying this formula the matrix elements for d^4 (including spin–orbit coupling interaction) have been calculated and tabulated.

In the case of a transition-metal ion embedded in a weak octahedral crystalline field, the spin–orbit coupling and the crystal-field interactions can be treated as a perturbation, using $|LSJM\rangle$ as the basis functions.[1] This perturba-

TABLE I. Nonvanishing matrix elements of $(d^4v'L'S'J'\Gamma_1 | \mathcal{H}' | d^4vLSJ\Gamma_1)$.

$v'L'S'J'$	$vLSJ$	Dq	ζ_{nd}	$v'L'S'J'$	$vLSJ$	Dq	ζ_{nd}
$^5_4D_4$	$^5_4D_4$	-2	1	$^3_4G_4$	$^1_4G_4$	0	$(33)^{1/2}/6$
$^5_4D_4$	$^5_4D_0$	$-2(6)^{1/2}$	0	$^3_2F_4$	$^3_2F_4$	-2	$1/2$
$^5_4D_4$	$^3_2F_4$	0	$\sqrt{2}$	$^3_2F_4$	$^3_4F_4$	0	$-1/2$
$^5_4D_4$	$^3_4F_4$	0	$-\sqrt{2}$	$^3_2F_4$	$^3_2P_0$	$-4/3$	0
$^5_4D_0$	$^5_4D_0$	0	$-3/2$	$^3_2F_4$	$^3_4P_0$	$20(14)^{1/2}/21$	0
$^5_4D_0$	$^3_2P_0$	0	$4\sqrt{3}/3$	$^3_2F_4$	$^1_2G_4$	0	$1/3$
$^5_4D_0$	$^3_4P_0$	0	$-(42)^{1/2}/6$	$^3_2F_4$	$^1_4G_4$	0	$-(11)^{1/2}/3$
$^3_4H_6$	$^3_4H_6$	$-56/11$	$1/2$	$^3_4F_4$	$^3_4F_4$	3	$-1/4$
$^3_4H_6$	$^3_4H_4$	$-16(35)^{1/2}/77$	0	$^3_4F_4$	$^3_2P_0$	$20/3$	0
$^3_4H_6$	$^3_4G_4$	$3(2310)^{1/2}/77$	0	$^3_4F_4$	$^3_4P_0$	$-(14)^{1/2}/21$	0
$^3_4H_6$	$^3_2F_4$	$-20(770)^{1/2}/77$	0	$^3_4F_4$	$^1_2G_4$	0	$-5/3$
$^3_4H_6$	$^3_4F_4$	$15(770)^{1/2}/77$	0	$^3_4F_4$	$^1_4G_4$	0	$(11)^{1/2}/6$
$^3_4H_6$	$^1_4I_6$	0	$(6)^{1/2}/2$	$^3_2P_0$	$^3_2P_0$	0	$-1/3$
$^3_4H_4$	$^3_4H_4$	$56/11$	$-3/5$	$^3_2P_0$	$^3_4P_0$	0	$2(14)^{1/2}/3$
$^3_4H_4$	$^3_4G_4$	$7(66)^{1/2}/33$	$-2(66)^{1/2}/15$	$^3_2P_0$	$^1_0S_0$	0	-3
$^3_4H_4$	$^3_2F_4$	$4(22)^{1/2}/11$	0	$^3_2P_0$	$^1_4S_0$	0	$(21)^{1/2}/3$
$^3_4H_4$	$^3_4F_4$	$-3(22)^{1/2}/11$	0	$^3_4P_0$	$^3_4P_0$	0	$-2/3$
$^3_4H_4$	$^3_2P_0$	$-4(22)^{1/2}/3$	0	$^3_4P_0$	$^1_4S_0$	0	$-2(6)^{1/2}/3$
$^3_4H_4$	$^3_4P_0$	$4(77)^{1/2}/21$	0	$^1_4I_6$	$^1_4I_6$	$84/11$	0
$^3_4H_4$	$^1_2G_4$	0	$(22)^{1/2}/3$	$^1_4I_6$	$^1_2G_4$	$-80(1155)^{1/2}/231$	0
$^3_4H_4$	$^1_4G_4$	0	$-2\sqrt{2}/3$	$^1_4I_6$	$^1_4G_4$	$100(105)^{1/2}/231$	0
$^3_4G_4$	$^3_4G_4$	-3	$-3/20$	$^1_2G_4$	$^1_2G_4$	$4/3$	0
$^3_4G_4$	$^3_2F_4$	$8\sqrt{3}/3$	$-5\sqrt{3}/6$	$^1_2G_4$	$^1_4G_4$	$-80(11)^{1/2}/33$	0
$^3_4G_4$	$^3_4F_4$	$-\sqrt{3}/3$	$5\sqrt{3}/12$	$^1_2G_4$	$^1_0S_0$	12	0
$^3_4G_4$	$^3_2P_0$	$4\sqrt{3}/3$	0	$^1_2G_4$	$^1_4S_0$	$-20(21)^{1/2}/21$	0
$^3_4G_4$	$^3_4P_0$	$-17(42)^{1/2}/21$	0	$^1_4G_4$	$^1_4G_4$	$34/33$	0
$^3_4G_4$	$^1_2G_4$	0	$\sqrt{3}/3$	$^1_4G_4$	$^1_4S_0$	$8(231)^{1/2}/21$	0

TABLE II. Nonvanishing matrix elements of $(d^4v'L'S'J'\Gamma_2 | \mathcal{H}' | d^4vLSJ\Gamma_2)$.

$v'L'S'J'$	$vLSJ$	Dq	ζ_{nd}	$v'L'S'J'$	$vLSJ$	Dq	ζ_{nd}
$^5_4D_3$	$^5_4D_3$	-6	0	$^3_4G_3$	$^1_4F_3$	0	$3(21)^{1/2}/14$
$^5_4D_3$	$^3_2F_3$	0	$(6)^{1/2}/3$	$^3_2F_3$	$^3_2F_3$	$2/3$	$-1/6$
$^5_4D_3$	$^3_4F_3$	0	$-(6)^{1/2}/3$	$^3_2F_3$	$^3_4F_3$	0	$1/6$
$^5_4D_3$	$^3_4D_3$	0	$(42)^{1/2}/6$	$^3_2F_3$	$^3_4D_3$	$40(7)^{1/2}/21$	$-10(7)^{1/2}/21$
$^3_4H_6$	$^3_4H_6$	$8/3$	$1/2$	$^3_2F_3$	$^1_4F_3$	0	$(15)^{1/2}/3$
$^3_4H_6$	$^3_4G_3$	$-(14)^{1/2}i/7$	0	$^3_4F_3$	$^3_4F_3$	-1	$1/12$
$^3_4H_6$	$^3_2F_3$	$4(10)^{1/2}i/3$	0	$^3_4F_3$	$^3_4D_3$	$10(7)^{1/2}/7$	$-2(7)^{1/2}/21$
$^3_4H_6$	$^3_4F_3$	$-(10)^{1/2}i$	0	$^3_4F_3$	$^1_4F_3$	0	$(15)^{1/2}/6$
$^3_4H_6$	$^3_4D_3$	$8(70)^{1/2}i/21$	0	$^3_4D_3$	$^3_4D_3$	$44/21$	$-1/6$
$^3_4H_6$	$^1_4I_6$	0	$(6)^{1/2}/2$	$^3_4D_3$	$^1_4F_3$	0	$2(105)^{1/2}/21$
$^3_4G_3$	$^3_4G_3$	$39/7$	$-3/4$	$^1_4I_6$	$^1_4I_6$	-4	0
$^3_4G_3$	$^3_2F_3$	$-8(35)^{1/2}/7$	$-3(35)^{1/2}/14$	$^1_4I_6$	$^1_4F_3$	$-4i$	0
$^3_4G_3$	$^3_4F_3$	$(35)^{1/2}/7$	$3(35)^{1/2}/28$	$^1_4F_3$	$^1_4F_3$	2	0
$^3_4G_3$	$^3_4D_3$	$-6(5)^{1/2}/7$	0				

[1] A. D. Liehr and C. J. Ballhausen, Ann. Phys. (N.Y.) 6, 134 (1959).

TABLE III. Nonvanishing matrix elements of $(d^4v'L'S'J'\Gamma_3 \mid \mathcal{H}' \mid d^4vLSJ\Gamma_3)$.

$v'L'S'J'$	$vLSJ$	Dq	ζ_{nd}
${}^5_4D_4$	${}^5_4D_4$	$-2/7$	1
${}^5_4D_4$	${}^5_4D_2$	$-20\sqrt{3}/7$	0
${}^5_4D_4$	${}^3_2F_4$	0	$\sqrt{2}$
${}^5_4D_4$	${}^3_4F_4$	0	$-\sqrt{2}$
${}^5_4D_2$	${}^5_4D_2$	$-12/7$	$-3/4$
${}^5_4D_2$	${}^3_2F_2$	0	$(30)^{1/2}/15$
${}^5_4D_2$	${}^3_4F_2$	0	$-(30)^{1/2}/15$
${}^5_4D_2$	${}^3_4D_2$	0	$7\sqrt{3}/12$
${}^5_4D_2$	${}^3_2P_2$	0	$2(105)^{1/2}/15$
${}^5_4D_2$	${}^3_4P_2$	0	$-7(30)^{1/2}/60$
${}^3_4H_6$	${}^3_4H_6$	$152/33$	$1/2$
${}^3_4H_6$	${}^3_4H_5$	$8(22)^{1/2}i/33$	0
${}^3_4H_6$	${}^3_4H_4$	$16(7)^{1/2}/77$	0
${}^3_4H_6$	${}^3_4G_5$	$-2(22)^{1/2}i/11$	0
${}^3_4H_6$	${}^3_4G_4$	$-3(462)^{1/2}/77$	0
${}^3_4H_6$	${}^3_2F_4$	$20(154)^{1/2}/77$	0
${}^3_4H_6$	${}^3_2F_2$	$8(770)^{1/2}/231$	0
${}^3_4H_6$	${}^3_4F_4$	$-15(154)^{1/2}/77$	0
${}^3_4H_6$	${}^3_4F_2$	$-2(770)^{1/2}/77$	0
${}^3_4H_6$	${}^3_4D_2$	$40(77)^{1/2}/231$	0
${}^3_4H_6$	${}^3_2P_2$	$-8(55)^{1/2}/11$	0
${}^3_4H_6$	${}^3_4P_2$	$4(770)^{1/2}/77$	0
${}^3_4H_6$	${}^1_4I_6$	0	$(6)^{1/2}/2$
${}^3_4H_5$	${}^3_4H_5$	$-8/3$	$-1/10$
${}^3_4H_5$	${}^3_4H_4$	$-24(154)^{1/2}i/77$	0
${}^3_4H_5$	${}^3_4G_5$	-1	$-6/5$
${}^3_4H_5$	${}^3_4G_4$	$3(21)^{1/2}i/7$	0
${}^3_4H_5$	${}^3_2F_4$	$12(7)^{1/2}i/7$	0
${}^3_4H_5$	${}^3_2F_2$	$52(35)^{1/2}i/105$	0
${}^3_4H_5$	${}^3_4F_4$	$-9(7)^{1/2}i/7$	0
${}^3_4H_5$	${}^3_4F_2$	$-13(35)^{1/2}i/35$	0
${}^3_4H_5$	${}^3_4D_2$	$8(14)^{1/2}i/21$	0
${}^3_4H_5$	${}^3_2P_2$	$4(10)^{1/2}i/5$	0
${}^3_4H_5$	${}^3_4P_2$	$-4(35)^{1/2}i/35$	0
${}^3_4H_4$	${}^3_4H_4$	$8/11$	$-3/5$
${}^3_4H_4$	${}^3_4G_5$	$4(154)^{1/2}i/77$	0
${}^3_4H_4$	${}^3_4G_4$	$(66)^{1/2}/33$	$-2(66)^{1/2}/15$
${}^3_4H_4$	${}^3_2F_4$	$4(22)^{1/2}/77$	0
${}^3_4H_4$	${}^3_2F_2$	$208(110)^{1/2}/385$	0
${}^3_4H_4$	${}^3_4F_4$	$-3(22)^{1/2}/77$	0
${}^3_4H_4$	${}^3_4F_2$	$-156(110)^{1/2}/385$	0
${}^3_4H_4$	${}^3_4D_2$	$-8(11)^{1/2}/11$	0
${}^3_4H_4$	${}^3_2P_2$	$-16(385)^{1/2}/165$	0
${}^3_4H_4$	${}^3_4P_2$	$8(110)^{1/2}/165$	0
${}^3_4H_4$	${}^1_2G_4$	0	$(22)^{1/2}/3$
${}^3_4H_4$	${}^1_4G_4$	0	$-2\sqrt{2}/3$
${}^3_4G_5$	${}^3_4G_5$	3	$3/5$
${}^3_4G_5$	${}^3_4G_4$	$6(21)^{1/2}i/7$	0
${}^3_4G_5$	${}^3_2F_4$	$16(7)^{1/2}i/7$	0
${}^3_4G_5$	${}^3_2F_2$	$-8(35)^{1/2}i/35$	0
${}^3_4G_5$	${}^3_4F_4$	$-2(7)^{1/2}i/7$	0
${}^3_4G_5$	${}^3_4F_2$	$(35)^{1/2}i/35$	0
${}^3_4G_5$	${}^5_4D_2$	$3(14)^{1/2}i/7$	0
${}^3_4G_5$	${}^3_2P_2$	$2(10)^{1/2}i/5$	0
${}^3_4G_5$	${}^3_4P_2$	$-17(35)^{1/2}i/35$	0
${}^3_4G_4$	${}^3_4G_4$	$-3/7$	$-3/20$
${}^3_4G_4$	${}^3_2F_4$	$8\sqrt{3}/21$	$-5\sqrt{3}/6$
${}^3_4G_4$	${}^3_2F_2$	$-48(15)^{1/2}/35$	0
${}^3_4G_4$	${}^3_4F_4$	$-\sqrt{3}/21$	$5\sqrt{3}/12$
${}^3_4G_4$	${}^3_4F_2$	$6(15)^{1/2}/35$	0
${}^3_4G_4$	${}^3_4D_2$	$3(6)^{1/2}/7$	0
${}^3_4G_4$	${}^3_2P_2$	$-2(210)^{1/2}/15$	0
${}^3_4G_4$	${}^3_4P_2$	$17(15)^{1/2}/15$	0
${}^3_4G_4$	${}^1_2G_4$	0	$\sqrt{3}/3$
${}^3_4G_4$	${}^1_4G_4$	0	$(33)^{1/2}/6$
${}^3_2F_4$	${}^3_2F_4$	$-2/7$	$1/2$
${}^3_2F_4$	${}^3_2F_2$	$-4(5)^{1/2}/7$	0
${}^3_2F_4$	${}^3_4F_4$	0	$-1/2$
${}^3_2F_4$	${}^3_4D_2$	$20\sqrt{2}/7$	0
${}^3_2F_4$	${}^3_2P_2$	$-2(70)^{1/2}/21$	0
${}^3_2F_4$	${}^3_4P_2$	$20(5)^{1/2}/21$	0
${}^3_2F_4$	${}^1_2G_4$	0	$1/3$
${}^3_2F_4$	${}^1_4G_4$	0	$-(11)^{1/2}/3$
${}^3_2F_2$	${}^3_2F_2$	$-22/21$	$-2/3$
${}^3_2F_2$	${}^3_4F_2$	0	$2/3$
${}^3_2F_2$	${}^3_4D_2$	$-20(10)^{1/2}/21$	$-(10)^{1/2}/3$
${}^3_2F_2$	${}^3_2P_2$	$-2(14)^{1/2}/7$	0
${}^3_2F_2$	${}^3_4P_2$	$20/7$	0
${}^3_2F_2$	${}^1_2D_2$	0	$-2(15)^{1/2}/15$
${}^3_2F_2$	${}^1_4D_2$	0	$-(30)^{1/2}/15$
${}^3_4F_4$	${}^3_4F_4$	$3/7$	$-1/4$
${}^3_4F_4$	${}^3_4F_2$	$6(5)^{1/2}/7$	0
${}^3_4F_4$	${}^3_4D_2$	$15\sqrt{2}/7$	0
${}^3_4F_4$	${}^3_2P_2$	$10(70)^{1/2}/21$	0
${}^3_4F_4$	${}^3_4P_2$	$-(5)^{1/2}/21$	0
${}^3_4F_4$	${}^1_2G_4$	0	$-5/3$
${}^3_4F_4$	${}^1_4G_4$	0	$(11)^{1/2}/6$
${}^3_4F_2$	${}^3_4F_2$	$11/7$	$1/3$
${}^3_4F_2$	${}^3_4D_2$	$-5(10)^{1/2}/7$	$-(10)^{1/2}/15$
${}^3_4F_2$	${}^3_2P_2$	$10(14)^{1/2}/7$	0
${}^3_4F_2$	${}^3_4P_2$	$-1/7$	0
${}^3_4F_2$	${}^1_2D_2$	0	$-4(15)^{1/2}/15$
${}^3_4F_2$	${}^1_4D_2$	0	$4(30)^{1/2}/15$
${}^3_4D_2$	${}^3_4D_2$	$44/21$	$1/12$
${}^3_4D_2$	${}^3_4P_2$	0	$-9(10)^{1/2}/20$
${}^3_4D_2$	${}^1_2D_2$	0	$2(6)^{1/2}/3$
${}^3_4D_2$	${}^1_4D_2$	0	$-\sqrt{3}/3$
${}^3_2P_2$	${}^3_2P_2$	0	$1/6$
${}^3_2P_2$	${}^3_4P_2$	0	$-(14)^{1/2}/3$
${}^3_2P_2$	${}^1_2D_2$	0	$(210)^{1/2}/30$
${}^3_2P_2$	${}^1_4D_2$	0	$-2(105)^{1/2}/15$
${}^3_4P_2$	${}^3_4P_2$	0	$1/3$
${}^3_4P_2$	${}^1_2D_2$	0	$-2(15)^{1/2}/15$
${}^3_4P_2$	${}^1_4D_2$	0	$-(30)^{1/2}/30$
${}^1_4I_6$	${}^1_4I_6$	$-76/11$	0
${}^1_4I_6$	${}^1_2G_4$	$80(231)^{1/2}/231$	0
${}^1_4I_6$	${}^1_4G_4$	$-100(21)^{1/2}/231$	0
${}^1_4I_6$	${}^1_2D_2$	$-40(77)^{1/2}/77$	0
${}^1_4I_6$	${}^1_4D_2$	$20(154)^{1/2}/77$	0
${}^1_2G_4$	${}^1_2G_4$	$4/21$	0
${}^1_2G_4$	${}^1_4G_4$	$-80(11)^{1/2}/231$	0
${}^1_2G_4$	${}^1_2D_2$	$40\sqrt{3}/21$	0
${}^1_2G_4$	${}^1_4D_2$	$-40(6)^{1/2}/21$	0
${}^1_4G_4$	${}^1_4G_4$	$34/231$	0
${}^1_4G_4$	${}^1_2D_2$	$40(33)^{1/2}/231$	0
${}^1_4G_4$	${}^1_4D_2$	$-130(66)^{1/2}/231$	0
${}^1_2D_2$	${}^1_2D_2$	$8/7$	0
${}^1_2D_2$	${}^1_4D_2$	$20\sqrt{2}/7$	0
${}^1_4D_2$	${}^1_4D_2$	$-32/7$	0

TABLE IV. Nonvanishing matrix elements of $(d^4v'L'S'J'\Gamma_4 | \mathcal{H}' | d^4vLSJ\Gamma_4)$.

$v'L'S'J'$	$vLSJ$	Dq	ζ_{nd}
$^5_4D_4$	$^5_4D_4$	-1	1
$^5_4D_4$	$^5_4D_3$	$(5)^{1/2}i$	0
$^5_4D_4$	$^5_4D_1$	$2(5)^{1/2}i$	0
$^5_4D_4$	$^3_2F_4$	0	$\sqrt{2}$
$^5_4D_4$	$^3_4F_4$	0	$-\sqrt{2}$
$^5_4D_3$	$^5_4D_3$	3	0
$^5_4D_3$	$^5_4D_1$	-2	0
$^5_4D_3$	$^3_2F_3$	0	$(6)^{1/2}/3$
$^5_4D_3$	$^3_4F_3$	0	$-(6)^{1/2}/3$
$^5_4D_3$	$^3_4D_3$	0	$(42)^{1/2}/6$
$^5_4D_1$	$^5_4D_1$	0	$-5/4$
$^5_4D_1$	$^3_4D_1$	0	$(7)^{1/2}/4$
$^5_4D_1$	$^3_2P_1$	0	2
$^5_4D_1$	$^3_4P_1$	0	$-(14)^{1/2}/4$
$^3_4H_6$	$^3_4H_6$	$-128/33$	$1/2$
$^3_4H_6$	$^3_4H_5$	$-4(385)^{1/2}i/33$	0
$^3_4H_6$	$^3_4H_5'$	$4(11)^{1/2}i/33$	0
$^3_4H_6$	$^3_4H_4$	$4(6)^{1/2}/11$	0
$^3_4H_6$	$^3_4G_5$	$(385)^{1/2}i/11$	0
$^3_4H_6$	$^3_4G_5'$	$-(11)^{1/2}i/11$	0
$^3_4H_6$	$^3_4G_4$	$-9(11)^{1/2}/22$	0
$^3_4H_6$	$^3_4G_3$	$5(77)^{1/2}i/154$	0
$^3_4H_6$	$^3_2F_4$	$10(33)^{1/2}/11$	0
$^3_4H_6$	$^3_2F_3$	$-10(55)^{1/2}i/33$	0
$^3_4H_6$	$^3_4F_4$	$-15(33)^{1/2}/22$	0
$^3_4H_6$	$^3_4F_3$	$5(55)^{1/2}i/22$	0
$^3_4H_6$	$^3_4D_3$	$-20(385)^{1/2}i/231$	0
$^3_4H_6$	$^1_4I_6$	0	$(6)^{1/2}/2$
$^3_4H_5$	$^3_4H_5$	$8/3$	$-1/10$
$^3_4H_5$	$^3_4H_5'$	$8(35)^{1/2}/21$	$-1/10$
$^3_4H_5$	$^3_4H_4$	$-4(2310)^{1/2}i/231$	0
$^3_4H_5$	$^3_4G_5$	1	$-6/5$
$^3_4H_5$	$^3_4G_5'$	$(35)^{1/2}/7$	$-6/5$
$^3_4H_5$	$^3_4G_4$	$(35)^{1/2}i/14$	0
$^3_4H_5$	$^3_4G_3$	$(5)^{1/2}/2$	0
$^3_4H_5$	$^3_2F_4$	$2(105)^{1/2}i/21$	0
$^3_4H_5$	$^3_2F_3$	$-22(7)^{1/2}/21$	0
$^3_4H_5$	$^3_4F_4$	$-(105)^{1/2}/14$	0
$^3_4H_5$	$^3_4F_3$	$11(7)^{1/2}/14$	0
$^3_4H_5$	$^3_4D_3$	$4/3$	0
$^3_4H_5$	$^3_4D_1$	$2(6)^{1/2}/3$	0
$^3_4H_5$	$^3_2P_1$	$-2(42)^{1/2}/3$	0
$^3_4H_5$	$^3_4P_1$	$2\sqrt{3}/3$	0
$^3_4H_5'$	$^3_4H_5'$	$-8/3$	$-1/10$
$^3_4H_5'$	$^3_4H_4$	$-4(66)^{1/2}i/11$	0
$^3_4H_5'$	$^3_4G_5$	$(35)^{1/2}/7$	$-6/5$
$^3_4H_5'$	$^3_4G_5'$	-1	$-6/5$
$^3_4H_5'$	$^3_4G_4$	$3i/2$	0
$^3_4H_5'$	$^3_4G_3$	$-(7)^{1/2}/2$	0
$^3_4H_5'$	$^3_2F_4$	$2\sqrt{3}i$	0
$^3_4H_5'$	$^3_2F_3$	$22(5)^{1/2}/15$	0
$^3_4H_5'$	$^3_4F_4$	$-3\sqrt{3}i/2$	0
$^3_4H_5'$	$^3_4F_3$	$-11(5)^{1/2}/10$	0
$^3_4H_5'$	$^3_4D_3$	$-4(35)^{1/2}/15$	0
$^3_4H_5'$	$^3_4D_1$	$2(210)^{1/2}/35$	0
$^3_4H_5'$	$^3_2P_1$	$-2(30)^{1/2}/5$	0
$^3_4H_5'$	$^3_4P_1$	$2(105)^{1/2}/35$	0
$^3_4H_4$	$^3_4H_4$	$28/11$	$-3/5$
$^3_4H_4$	$^3_4G_5$	$2(2310)^{1/2}i/693$	0
$^3_4H_4$	$^3_4G_5'$	$2(66)^{1/2}i/33$	0
$^3_4H_4$	$^3_4G_4$	$7(66)^{1/2}/66$	$-2(66)^{1/2}/15$
$^3_4H_4$	$^3_4G_3$	$13(462)^{1/2}i/198$	0
$^3_4H_4$	$^3_2F_4$	$2(22)^{1/2}/11$	0
$^3_4H_4$	$^3_2F_3$	$26(330)^{1/2}i/165$	0
$^3_4H_4$	$^3_4F_4$	$-3(22)^{1/2}/22$	0
$^3_4H_4$	$^3_4F_3$	$-13(330)^{1/2}i/110$	0
$^3_4H_4$	$^3_4D_3$	$-2(2310)^{1/2}i/165$	0
$^3_4H_4$	$^3_4D_1$	$-4(385)^{1/2}i/35$	0
$^3_4H_4$	$^3_2P_1$	$-8(55)^{1/2}i/15$	0
$^3_4H_4$	$^3_4P_1$	$-4(770)^{1/2}i/105$	0
$^3_4H_4$	$^1_2G_4$	0	$(22)^{1/2}/3$
$^3_4H_4$	$^1_4G_4$	0	$-2\sqrt{2}/3$
$^3_4G_5$	$^3_4G_5$	-3	$3/5$
$^3_4G_5$	$^3_4G_5'$	$-3(35)^{1/2}/7$	$3/5$
$^3_4G_5$	$^3_4G_4$	$(35)^{1/2}i/7$	0
$^3_4G_5$	$^3_4G_3$	$3(5)^{1/2}/7$	0
$^3_4G_5$	$^3_2F_4$	$8(105)^{1/2}i/63$	0
$^3_4G_5$	$^3_2F_3$	$8(7)^{1/2}/7$	0
$^3_4G_5$	$^3_4F_4$	$-(105)^{1/2}i/63$	0
$^3_4G_5$	$^3_4F_3$	$-(7)^{1/2}/7$	0
$^3_4G_5$	$^3_4D_3$	$-12/7$	0
$^3_4G_5$	$^3_4D_1$	$(6)^{1/2}/3$	0
$^3_4G_5$	$^3_2P_1$	$2(42)^{1/2}/9$	0
$^3_4G_5$	$^3_4P_1$	$-17\sqrt{3}/9$	0
$^3_4G_5'$	$^3_4G_5'$	3	$3/5$
$^3_4G_5'$	$^3_4G_4$	$3i$	0
$^3_4G_5'$	$^3_4G_3$	$-3(7)^{1/2}/7$	0
$^3_4G_5'$	$^3_2F_4$	$8\sqrt{3}i/3$	0
$^3_4G_5'$	$^3_2F_3$	$-8(5)^{1/2}/5$	0
$^3_4G_5'$	$^3_4F_4$	$-\sqrt{3}i/3$	0
$^3_4G_5'$	$^3_4F_3$	$(5)^{1/2}/5$	0
$^3_4G_5'$	$^3_4D_3$	$12(35)^{1/2}/35$	0
$3_4G_5'$	$^3_4D_1$	$(210)^{1/2}/35$	0
$^3_4G_5'$	$^3_2P_1$	$2(30)^{1/2}/15$	0
$^3_4G_5'$	$^3_4P_1$	$-17(105)^{1/2}/105$	0
$^3_4G_4$	$^3_4G_4$	$-3/2$	$-3/20$
$^3_4G_4$	$^3_4G_3$	$13(7)^{1/2}i/14$	0
$^3_4G_4$	$^3_2F_4$	$4\sqrt{3}/3$	$-5\sqrt{3}/6$
$^3_4G_4$	$^3_2F_3$	$4(5)^{1/2}i/5$	0
$^3_4G_4$	$^3_4F_4$	$-\sqrt{3}/6$	$5\sqrt{3}/12$
$^3_4G_4$	$^3_4F_3$	$-(5)^{1/2}i/10$	0
$^3_4G_4$	$^3_4D_3$	$9(35)^{1/2}i/35$	0
$^3_4G_4$	$^3_4D_1$	$-11(210)^{1/2}i/70$	0
$^3_4G_4$	$^3_2P_1$	$-(30)^{1/2}i/15$	0
$^3_4G_4$	$^3_4P_1$	$17(105)^{1/2}i/210$	0
$^3_4G_4$	$^1_2G_4$	0	$\sqrt{3}/3$
$^3_4G_4$	$^1_4G_4$	0	$(33)^{1/2}/6$
$^3_4G_3$	$^3_4G_3$	$-33/14$	$-3/4$
$^3_4G_3$	$^3_2F_4$	$20(21)^{1/2}i/63$	0
$^3_4G_3$	$^3_2F_3$	$4(35)^{1/2}/7$	$-3(35)^{1/2}/14$
$^3_4G_3$	$^3_4F_4$	$-5(21)^{1/2}i/126$	0
$^3_4G_3$	$^3_4F_3$	$-(35)^{1/2}/14$	$3(35)^{1/2}/28$
$^3_4G_3$	$^3_4D_3$	$3(5)^{1/2}/7$	0
$^3_4G_3$	$^3_4D_1$	$-11(30)^{1/2}/42$	0
$^3_4G_3$	$^3_2P_1$	$(210)^{1/2}/9$	0
$^3_4G_3$	$^3_4P_1$	$-17(15)^{1/2}/18$	0

TABLE IV (*Continued*)

$v'L'S'J'$	$vLSJ$	Dq	ζ_{nd}	$v'L'S'J'$	$vLSJ$	Dq	ζ_{nd}
${}^3_4G_3$	${}^1_4F_3$	0	$3(21)^{1/2}/14$	${}^3_4F_4$	${}^1_4G_4$	0	$(11)^{1/2}/6$
${}^3_2F_4$	${}^3_2F_4$	-1	$1/2$	${}^3_4F_3$	${}^3_4F_3$	$1/2$	$1/12$
${}^3_2F_4$	${}^3_2F_3$	$(15)^{1/2}i/3$	0	${}^3_4F_3$	${}^3_4D_3$	$-5(7)^{1/2}/7$	$-2(7)^{1/2}/21$
${}^3_2F_4$	${}^3_4F_4$	0	$-1/2$	${}^3_4F_3$	${}^3_4D_1$	$-5(42)^{1/2}/14$	0
${}^3_2F_4$	${}^3_4D_3$	$-4(105)^{1/2}i/21$	0	${}^3_4F_3$	${}^3_2P_1$	$5(6)^{1/2}/3$	0
${}^3_2F_4$	${}^3_4D_1$	$-2(70)^{1/2}i/7$	0	${}^3_4F_3$	${}^3_4P_1$	$-(21)^{1/2}/42$	0
${}^3_2F_4$	${}^3_2P_1$	$(10)^{1/2}i/3$	0	${}^3_4F_3$	${}^1_4F_3$	0	$(15)^{1/2}/6$
${}^3_2F_4$	${}^3_4P_1$	$-10(35)^{1/2}i/21$	0	3_4D_3	${}^3_4D_3$	$22/21$	$-1/6$
${}^3_2F_4$	${}^1_2G_4$	0	$1/3$	${}^3_4D_3$	${}^3_4D_1$	$22(6)^{1/2}/21$	0
${}^3_2F_4$	${}^1_4G_4$	0	$-(11)^{1/2}/3$	${}^3_4D_3$	${}^1_4F_3$	0	$2(105)^{1/2}/21$
${}^3_2F_3$	${}^2_2F_3$	$-1/3$	$-1/6$	${}^3_4D_1$	${}^3_4D_1$	0	$1/4$
${}^3_2F_3$	${}^3_4F_3$	0	$1/6$	${}^3_4D_1$	${}^3_4P_1$	0	$-3\sqrt{2}/4$
${}^3_2F_3$	${}^3_4D_3$	$-20(7)^{1/2}/21$	$-10(7)^{1/2}/21$	${}^3_2P_1$	${}^3_2P_1$	0	$-1/6$
${}^3_2F_3$	${}^3_4D_1$	$-10(42)^{1/2}/21$	0	${}^3_2P_1$	${}^3_4P_1$	0	$(14)^{1/2}/3$
${}^3_2F_3$	${}^3_2P_1$	$-(6)^{1/2}/3$	0	${}^3_4P_1$	${}^3_4P_1$	0	$-1/3$
${}^3_2F_3$	${}^3_4P_1$	$10(21)^{1/2}/21$	0	${}^1_4I_6$	${}^1_4I_6$	$64/11$	0
${}^3_2F_3$	${}^1_4F_3$	0	$(15)^{1/2}/3$	${}^1_4I_6$	${}^1_2G_4$	$20(22)^{1/2}/21$	0
${}^3_4F_4$	${}^3_4F_4$	$3/2$	$-1/4$	${}^1_4I_6$	${}^1_4G_4$	$-25\sqrt{2}/11$	0
${}^3_4F_4$	${}^3_4F_3$	$-(15)^{1/2}i/2$	0	${}^1_4I_6$	${}^1_4F_3$	$5(22)^{1/2}i/11$	0
${}^3_4F_4$	${}^3_4D_3$	$-(105)^{1/2}i/7$	0	${}^1_2G_4$	${}^1_2G_4$	$2/3$	0
${}^3_4F_4$	${}^3_4D_1$	$-3(70)^{1/2}i/14$	0	${}^1_2G_4$	${}^1_4G_4$	$-40(11)^{1/2}/33$	0
${}^3_4F_4$	${}^3_2P_1$	$-5(10)^{1/2}i/3$	0	${}^1_4G_4$	${}^1_4G_4$	$17/33$	0
${}^3_4F_4$	${}^3_4P_1$	$(35)^{1/2}i/42$		${}^1_4G_4$	${}^1_4F_3$	$15(11)^{1/2}i/11$	0
${}^3_4F_4$	${}^1_2G_4$	0	$-5/3$	${}^1_4F_3$	${}^1_4F_3$	-1	0

tion Hamiltonian can be written as[2]

$$\mathcal{H}'=\zeta_{nd}\sum_i \mathbf{l}_i\cdot\mathbf{s}_i+(35Ze^2/4a^5)\sum_i(x_i^4+y_i^4+z_i^4-\tfrac{3}{5}r_i^4), \tag{1}$$

where ζ_{nd} is the one-electron spin–orbit coupling parameter and a is the effective distance between the ligand and the central ion.

The matrix elements $(d^nv'L'S'J'M'|\zeta_{nl,}\sum_i \mathbf{l}_i\cdot\mathbf{s}_i|d^nvLSJM)$ (where v is the seniority number, defined by Racah[3]) have been evaluated by Racah using irreducible tensor operator methods and have the form[3]

$$(d^nv'L'S'J'M'|\zeta_{nd}\sum_i \mathbf{l}_i\cdot\mathbf{s}_i|d^nvLSJM)=(-1)^{S'+L-J'}(30)^{1/2}(d^nv'L'S'||V^{(11)}||d^nvLS)$$
$$\times W(S'L'SL;J1)\delta_{JJ'}\delta_{MM'}\zeta_{nd} \tag{2}$$

The reduced matrix elements $(d^nv'L'S'\,||\,V^{(11)}\,||\,d^nvLS)$ are tabulated in numerous books[4] and the coefficients $W(abcd;ef)$ are the usual Racah coefficients.

In order to employ the powerful Racah algebra to evaluate the matrix elements of the octahedral crystal field, the potential is rewritten in terms of spherical harmonics,

$$\begin{aligned}V_{\text{oct}}&=(35Ze^2/4a^5)\sum_i(x_i^4+y_i^4+z_i^4-\tfrac{3}{5}r_i^4)\\&=(7Ze^2/3a^5)\pi^{1/2}\sum_i r_i^4\{Y_{40}(\theta_i,\varphi_i)+(5/14)^{1/2}[Y_{44}(\theta_i,\varphi_i)+Y_{4-4}(\theta_i,\varphi_i)]\}\\&=(4/15)D\pi^{1/2}\sum_i r_i^4\{Y_{40}(\theta_i,\varphi_i)+(5/14)^{1/2}[Y_{44}(\theta_i,\varphi_i)+Y_{4-4}(\theta_i,\varphi_i)]\},\end{aligned} \tag{3}$$

where

$$D=35Ze^2/4a^5. \tag{4}$$

Let $V_{kp}=\sum_i Y_{kp}(\theta_i,\varphi_i)$, then the matrix elements $(d^nv'L'S'J'M'\,|\,V_{kp}\,|\,d^nvLSJM)$ can be calculated in the

[2] T. M. Dunn, D. S. McClure, and R. G. Pearson, *Some Aspects of Crystal Field Theory* (Harper and Row, Publishers, Inc., New York, 1965), p. 12.
[3] G. Racah, Phys. Rev. 63, 367 (1943).
[4] J. C. Slater, *Quantum Theory of Atomic Structure* (McGraw-Hill Book Co., New York, 1960), Vol. 2, Appendix 26.

TABLE V. Nonvanishing matrix elements of $(d^4v'L'S'J'\Gamma_5\,|\,\mathcal{H}'\,|\,d^4vLSJ\Gamma_5)$.

$v'L'S'J'$	$vLSJ$	Dq	ζ_{nd}
${}^5_4D_4$	${}^5_4D_4$	$13/7$	1
${}^5_4D_4$	${}^5_4D_3$	$5(21)^{1/2}i/7$	0
${}^5_4D_4$	${}^5_4D_2$	$-10\sqrt{3}/7$	0
${}^5_4D_4$	${}^3_2F_4$	0	$\sqrt{2}$
${}^5_4D_4$	${}^3_4F_4$	0	$-\sqrt{2}$
${}^5_4D_3$	${}^5_4D_3$	-1	0
${}^5_4D_3$	${}^5_4D_2$	$-10(7)^{1/2}i/7$	0
${}^5_4D_3$	${}^3_2F_3$	0	$(6)^{1/2}/3$
${}^5_4D_3$	${}^3_4F_3$	0	$-(6)^{1/2}/3$
${}^5_4D_3$	${}^3_4D_3$	0	$(42)^{1/2}/6$
${}^5_4D_2$	${}^5_4D_2$	$8/7$	$-3/4$
${}^5_4D_2$	${}^3_2F_2$	0	$(30)^{1/2}/15$
${}^5_4D_2$	${}^3_4F_2$	0	$-(30)^{1/2}/15$
${}^5_4D_2$	${}^3_4D_2$	0	$7\sqrt{3}/12$
${}^5_4D_2$	${}^3_2P_2$	0	$2(105)^{1/2}/15$
${}^5_4D_2$	${}^3_4P_2$	0	$-7(30)^{1/2}/60$
${}^3_4H_6$	${}^3_4H_6$	$-236/99$	$1/2$
${}^3_4H_6$	${}^3_4H_6'$	$4(55)^{1/2}/33$	$1/2$
${}^3_4H_6$	${}^3_4H_5$	$-34(110)^{1/2}i/99$	0
${}^3_4H_6$	${}^3_4H_4$	$-4(35)^{1/2}/77$	0
${}^3_4H_6$	${}^3_4G_5$	$17(110)^{1/2}i/66$	0
${}^3_4H_6$	${}^3_4G_4$	$3(2310)^{1/2}/308$	0
${}^3_4H_6$	${}^3_4G_3$	$-23(154)^{1/2}i/924$	0
${}^3_4H_6$	${}^3_2F_4$	$-5(770)^{1/2}/77$	0
${}^3_4H_6$	${}^3_2F_3$	$23(110)^{1/2}i/99$	0
${}^3_4H_6$	${}^3_2F_2$	$26(154)^{1/2}/693$	0
${}^3_4H_6$	${}^3_4F_4$	$15(770)^{1/2}/308$	0
${}^3_4H_6$	${}^3_4F_3$	$-23(110)^{1/2}i/132$	0
${}^3_4H_6$	${}^3_4F_2$	$-13(154)^{1/2}/462$	0
${}^3_4H_6$	${}^3_4D_3$	$46(770)^{1/2}i/693$	0
${}^3_4H_6$	${}^3_4D_2$	$26(385)^{1/2}/693$	0
${}^3_4H_6$	${}^3_2P_2$	$-26(11)^{1/2}/33$	0
${}^3_4H_6$	${}^3_4P_2$	$13(154)^{1/2}/231$	0
${}^3_4H_6$	${}^1_4I_6$	0	$(6)^{1/2}/2$
${}^3_4H_6$	${}^1_4I_6'$	0	$(6)^{1/2}/2$
${}^3_4H_6'$	${}^3_4H_6'$	4	$1/2$
${}^3_4H_6'$	${}^3_4H_5$	$-2\sqrt{2}i/3$	0
${}^3_4H_6'$	${}^3_4H_4$	$4(77)^{1/2}/77$	0
${}^3_4H_6'$	${}^3_5G_5$	$\sqrt{2}i/2$	0
${}^3_4H_6'$	${}^3_5G_4$	$-3(42)^{1/2}/28$	0
${}^3_4H_6'$	${}^3_5G_3$	$(70)^{1/2}i/28$	0
${}^3_4H_6'$	${}^3_2F_4$	$5(14)^{1/2}/7$	0
${}^3_4H_6'$	${}^3_2F_3$	$-5\sqrt{2}i/3$	0
${}^3_4H_6'$	${}^3_2F_2$	$2(70)^{1/2}/21$	0
${}^3_4H_6'$	${}^3_4F_4$	$-15(14)^{1/2}/28$	0
${}^3_4H_6'$	${}^3_4F_3$	$5\sqrt{2}i/4$	0
${}^3_4H_6'$	${}^3_4F_2$	$-(70)^{1/2}/14$	0
${}^3_4H_6'$	${}^3_4D_3$	$-10(14)^{1/2}i/21$	0
${}^3_4H_6'$	${}^3_4D_2$	$10(7)^{1/2}/21$	0
${}^3_4H_6'$	${}^3_2P_2$	$-2(5)^{1/2}$	0
${}^3_4H_6'$	${}^3_4P_2$	$(70)^{1/2}/7$	0
${}^3_4H_6'$	${}^1_4I_6$	0	$(6)^{1/2}/2$
${}^2_4H_6'$	${}^1_4I_6'$	0	$(6)^{1/2}/2$
${}^3_4H_5$	${}^3_4H_5$	$16/9$	$-1/10$
${}^3_4H_5$	${}^3_4H_4$	$4(154)^{1/2}i/77$	0
${}^3_4H_5$	${}^3_4G_5$	$2/3$	$-6/5$
${}^3_4H_5$	${}^3_4G_4$	$-(21)^{1/2}i/14$	0
${}^3_4H_5$	${}^3_4G_3$	$-(35)^{1/2}/6$	0
${}^3_4H_5$	${}^3_2F_4$	$-2(7)^{1/2}i/7$	0
${}^3_4H_5$	${}^3_2F_3$	$22/9$	0
${}^3_4H_5$	${}^3_2F_2$	$-208(35)^{1/2}i/315$	0
${}^3_4H_5$	${}^3_4F_4$	$3(7)^{1/2}i/14$	0
${}^3_4H_5$	${}^3_4F_3$	$-11/6$	0
${}^3_4H_5$	${}^3_4F_2$	$52(35)^{1/2}i/105$	0
${}^3_4H_5$	${}^3_4D_3$	$-4(7)^{1/2}/9$	0
${}^3_4H_5$	${}^3_4D_2$	$-32(14)^{1/2}i/63$	0
${}^3_4H_5$	${}^3_2P_2$	$-16(10)^{1/2}i/15$	0
${}^3_4H_5$	${}^3_4P_2$	$16(35)^{1/2}i/105$	0
${}^3_4H_4$	${}^3_4H_4$	$-52/11$	$-3/5$
${}^3_4H_4$	${}^3_4G_5$	$-2(154)^{1/2}i/231$	0
${}^3_4H_4$	${}^3_4G_4$	$-13(66)^{1/2}/66$	$-2(66)^{1/2}/15$
${}^3_4H_4$	${}^3_4G_3$	$13(110)^{1/2}i/66$	0
${}^3_4H_4$	${}^3_2F_4$	$-26(22)^{1/2}/77$	0
${}^3_4H_4$	${}^3_2F_3$	$26(154)^{1/2}i/77$	0
${}^3_4H_4$	${}^3_2F_2$	$104(110)^{1/2}/385$	0
${}^3_4H_4$	${}^3_4F_4$	$39(22)^{1/2}/154$	0
${}^3_4H_4$	${}^3_4F_3$	$-39(154)^{1/2}i/154$	0
${}^3_4H_4$	${}^3_4F_2$	$-78(110)^{1/2}/385$	0
${}^3_4H_4$	${}^3_4D_3$	$-2(22)^{1/2}i/11$	0
${}^3_4H_4$	${}^3_4D_2$	$-4(11)^{1/2}/11$	0
${}^3_4H_4$	${}^3_2P_2$	$-8(385)^{1/2}/165$	0
${}^3_4H_4$	${}^3_4P_2$	$4(110)^{1/2}/165$	0
${}^3_4H_4$	${}^1_2G_4$	0	$(22)^{1/2}/3$
${}^3_4H_4$	${}^1_4G_4$	0	$-2\sqrt{2}/3$
${}^3_4G_5$	${}^3_4G_5$	-2	$3/5$
${}^3_4G_5$	${}^3_4G_4$	$-(21)^{1/2}i/7$	0
${}^3_4G_5$	${}^3_4G_3$	$-(35)^{1/2}/7$	0
${}^3_4G_5$	${}^3_2F_4$	$-8(7)^{1/2}i/21$	0
${}^3_4G_5$	${}^3_2F_3$	$-8/3$	0
${}^3_4G_5$	${}^3_2F_2$	$32(35)^{1/2}i/105$	0
${}^3_4G_5$	${}^3_4F_4$	$(7)^{1/2}i/21$	0
${}^3_4G_5$	${}^3_4F_3$	$1/3$	0
${}^3_4G_5$	${}^3_4F_2$	$-4(35)^{1/2}i/105$	0
${}^3_4G_5$	${}^3_4D_3$	$4(7)^{1/2}/7$	0
${}^3_4G_5$	${}^3_4D_2$	$-4(14)^{1/2}i/7$	0
${}^3_4G_5$	${}^3_2P_2$	$-8(10)^{1/2}i/15$	0
${}^3_4G_5$	${}^3_4P_2$	$68(35)^{1/2}i/105$	0
${}^3_4G_4$	${}^3_4G_4$	$39/14$	$-3/20$
${}^3_4G_4$	${}^3_4G_3$	$13(15)^{1/2}i/14$	0
${}^3_4G_4$	${}^3_2F_4$	$-52\sqrt{3}/21$	$-5\sqrt{3}/6$
${}^3_4G_4$	${}^3_2F_3$	$4(21)^{1/2}i/7$	0
${}^3_4G_4$	${}^3_2F_2$	$-24(15)^{1/2}/35$	0
${}^3_4G_4$	${}^3_4F_4$	$13\sqrt{3}/42$	$5\sqrt{3}/12$
${}^3_4G_4$	${}^3_4F_3$	$-(21)^{1/2}i/14$	0
${}^3_4G_4$	${}^3_4F_2$	$3(15)^{1/2}/35$	0
${}^3_4G_4$	${}^3_4D_3$	$9\sqrt{3}i/7$	0
${}^3_4G_4$	${}^3_4D_2$	$3(6)^{1/2}/14$	0
${}^3_4G_4$	${}^3_2P_2$	$-(210)^{1/2}/15$	0
${}^3_4G_4$	${}^3_4P_2$	$17(15)^{1/2}/30$	0
${}^3_4G_4$	${}^1_2G_4$	0	$\sqrt{3}/3$
${}^3_4G_4$	${}^1_4G_4$	0	$(33)^{1/2}/6$
${}^3_4G_3$	${}^3_4G_3$	$13/14$	$-3/4$
${}^3_4G_3$	${}^3_2F_4$	$20(5)^{1/2}i/21$	0
${}^3_4G_3$	${}^3_2F_3$	$-4(35)^{1/2}/21$	$-3(35)^{1/2}/14$
${}^3_4G_3$	${}^3_2F_2$	$88i/21$	0
${}^3_4G_3$	${}^3_4F_4$	$-5(5)^{1/2}i/42$	0
${}^3_4G_3$	${}^3_4F_3$	$(35)^{1/2}/42$	$3(35)^{1/2}/28$
${}^3_4G_3$	${}^3_4F_2$	$-11i/22$	0

TABLE V (*Continued*)

$v'L'S'J'$	$vLSJ$	Dq	ζ_{nd}	$v'L'S'J'$	$vLSJ$	Dq	ζ_{nd}
${}^3_4G_3$	${}^3_4D_3$	$-(5)^{1/2}/7$	0	${}^3_4F_2$	${}^3_4D_3$	$-20(5)^{1/2}i/21$	0
${}^3_4G_3$	${}^3_4D_2$	$11(10)^{1/2}i/14$	0	${}^3_4F_2$	${}^3_4D_2$	$10(10)^{1/2}/21$	$-(10)^{1/2}/15$
${}^3_4G_3$	${}^3_2P_2$	$-(14)^{1/2}i/3$	0	${}^3_4F_2$	${}^3_2P_2$	$-20(14)^{1/2}/21$	0
${}^3_4G_3$	${}^3_4P_2$	$17i/6$	0	${}^3_4F_2$	${}^3_4P_2$	$2/21$	0
${}^3_4G_3$	${}^1_4F_3$	0	$3(21)^{1/2}/14$	${}^3_4F_2$	${}^1_2D_2$	0	$-4(15)^{1/2}/15$
${}^3_2F_4$	${}^3_2F_4$	$13/7$	$1/2$	${}^3_4F_2$	${}^1_4D_2$	0	$4(30)^{1/2}/15$
${}^3_2F_4$	${}^3_2F_3$	$5(7)^{1/2}i/7$	0	${}^3_4D_3$	${}^3_4D_3$	$22/63$	$-1/6$
${}^3_2F_4$	${}^3_2F_2$	$-2(5)^{1/2}/7$	0	${}^3_4D_3$	${}^3_4D_2$	$110\sqrt{2}i/63$	0
${}^3_2F_4$	${}^3_4F_4$	0	$-1/2$	${}^3_4D_3$	${}^1_4F_3$	0	$2(105)^{1/2}/21$
${}^3_2F_4$	${}^3_4D_3$	$-20i/7$	0	${}^3_4D_2$	${}^3_4D_2$	$-88/63$	$1/12$
${}^3_2F_4$	${}^3_4D_2$	$10\sqrt{2}/7$	0	${}^3_4D_2$	${}^3_4P_2$	0	$-9(10)^{1/2}/20$
${}^3_2F_4$	${}^3_2P_2$	$-(70)^{1/2}/21$	0	${}^3_4D_2$	${}^1_2D_2$	0	$2(6)^{1/2}/3$
${}^3_2F_4$	${}^3_4P_2$	$10(5)^{1/2}/21$	0	${}^3_4D_2$	${}^1_4D_2$	0	$-\sqrt{3}/3$
${}^3_2F_4$	${}^1_2G_4$	0	$1/3$	${}^3_2P_2$	${}^3_2P_2$	0	$1/6$
${}^3_2F_4$	${}^1_4G_4$	0	$-(11)^{1/2}/3$	${}^3_2P_2$	${}^3_4P_2$	0	$-(14)^{1/2}/3$
${}^3_2F_3$	${}^3_2F_3$	$1/9$	$-1/6$	${}^3_2P_2$	${}^1_2D_2$	0	$(210)^{1/2}/30$
${}^3_2F_3$	${}^3_2F_2$	$22(35)^{1/2}i/63$	0	${}^3_2P_2$	${}^1_4D_2$	0	$-2(105)^{1/2}/15$
${}^3_2F_3$	${}^3_4F_3$	0	$1/6$	${}^3_4P_2$	${}^3_4P_2$	0	$1/3$
${}^3_2F_3$	${}^3_4D_3$	$20(7)^{1/2}/63$	$-10(7)^{1/2}/21$	${}^3_4P_2$	${}^1_2D_2$	0	$-2(15)^{1/2}/15$
${}^3_2F_3$	${}^3_4D_2$	$10(14)^{1/2}i/63$	0	${}^3_4P_2$	${}^1_4D_2$	0	$-(30)^{1/2}/30$
${}^3_2F_3$	${}^3_2P_2$	$-(10)^{1/2}i/3$	0	${}^1_4I_6$	${}^1_4I_6$	$118/33$	0
${}^3_2F_3$	${}^3_4P_2$	$10(35)^{1/2}i/21$	0	${}^1_4I_6$	${}^1_4I_6'$	$-2(55)^{1/2}/11$	0
${}^3_2F_3$	${}^1_4F_3$	0	$(15)^{1/2}/3$	${}^1_4I_6$	${}^1_2G_4$	$-20(1155)^{1/2}/231$	0
${}^3_2F_2$	${}^3_2F_2$	$44/63$	$-2/3$	${}^1_4I_6$	${}^1_4G_4$	$25(105)^{1/2}/231$	0
${}^3_2F_2$	${}^3_4F_2$	0	$2/3$	${}^1_4I_6$	${}^1_4F_3$	$-23(11)^{1/2}i/33$	0
${}^3_2F_2$	${}^3_4D_3$	$-80(5)^{1/2}i/63$	0	${}^1_4I_6$	${}^1_2D_2$	$-26(385)^{1/2}/231$	0
${}^3_2F_2$	${}^3_4D_2$	$40(10)^{1/2}/63$	$-(10)^{1/2}/3$	${}^1_4I_6$	${}^1_4D_2$	$13(770)^{1/2}/231$	0
${}^3_2F_2$	${}^3_2P_2$	$4(14)^{1/2}/21$	0	${}^1_4I_6'$	${}^1_4I_6'$	-6	0
${}^3_2F_2$	${}^3_4P_2$	$-40/21$	0	${}^1_4I_6'$	${}^1_2G_4$	$20(21)^{1/2}/21$	0
${}^3_2F_2$	${}^1_2D_2$	0	$-2(15)^{1/2}/15$	${}^1_4I_6'$	${}^1_4G_4$	$-25(231)^{1/2}/231$	0
${}^3_2F_2$	${}^1_4D_2$	0	$-(30)^{1/2}/15$	${}^1_4I_6'$	${}^1_4F_3$	$(5)^{1/2}i$	0
${}^3_4F_4$	${}^3_4F_4$	$-39/14$	$-1/4$	${}^1_4I_6'$	${}^1_2D_2$	$-10(7)^{1/2}/7$	0
${}^3_4F_4$	${}^3_4F_3$	$-15(7)^{1/2}i/14$	0	${}^1_4I_6'$	${}^1_4D_2$	$5(14)^{1/2}/7$	0
${}^3_4F_4$	${}^3_4F_2$	$3(5)^{1/2}/7$	0	${}^1_2G_4$	${}^1_2G_4$	$-26/21$	0
${}^3_4F_4$	${}^3_4D_3$	$-15i/7$	0	${}^1_2G_4$	${}^1_4G_4$	$520(11)^{1/2}/231$	0
${}^3_4F_4$	${}^3_4D_2$	$15\sqrt{2}/14$	0	${}^1_2G_4$	${}^1_2D_2$	$20\sqrt{3}/21$	0
${}^3_4F_4$	${}^3_2P_2$	$5(70)^{1/2}/21$	0	${}^1_2G_4$	${}^1_4D_2$	$-20(6)^{1/2}/21$	0
${}^3_4F_4$	${}^3_4P_2$	$-(5)^{1/2}/42$	0	${}^1_4G_4$	${}^1_4G_4$	$-221/231$	0
${}^3_4F_4$	${}^1_2G_4$	0	$-5/3$	${}^1_4G_4$	${}^1_4F_3$	$15(1155)^{1/2}i/77$	0
${}^3_4F_4$	${}^1_4G_4$	0	$(11)^{1/2}/6$	${}^1_4G_4$	${}^1_2D_2$	$20(33)^{1/2}/231$	0
${}^3_4F_3$	${}^3_4F_3$	$-1/6$	$1/12$	${}^1_4G_4$	${}^1_4D_2$	$-65(66)^{1/2}/231$	0
${}^3_4F_3$	${}^3_4F_2$	$-11(35)^{1/2}i/21$	0	${}^1_4F_3$	${}^1_4F_3$	$1/3$	0
${}^3_4F_3$	${}^3_4D_3$	$5(7)^{1/2}/21$	$-2(7)^{1/2}/21$	${}^1_4F_3$	${}^1_2D_2$	$-4(35)^{1/2}i/3$	0
${}^3_4F_3$	${}^3_4D_2$	$5(14)^{1/2}i/42$	0	${}^1_4F_3$	${}^1_4D_2$	$-(70)^{1/2}i/21$	0
${}^3_4F_3$	${}^3_2P_2$	$5(10)^{1/2}i/3$	0	${}^1_2D_2$	${}^1_2D_2$	$-16/21$	0
${}^3_4F_3$	${}^3_4P_2$	$-(35)^{1/2}i/42$	0	${}^1_2D_2$	${}^1_4D_2$	$-40\sqrt{2}/21$	0
${}^3_4F_3$	${}^1_4F_3$	0	$(15)^{1/2}/6$	${}^1_4D_4$	${}^1_4D_4$	$64/21$	0
${}^3_4F_2$	${}^3_4F_2$	$-22/21$	$1/3$				

following manner:

$$
\begin{aligned}
(d^n v' L'S'J'M' \mid V_{kp} \mid d^n vLSJM) &= \sum_{M_L(M_S)} \sum_{M_L'(M_S')} (LSM_LM_S \mid JM)(L'S'M_L'M_S' \mid J'M') \\
&\qquad \times (d^n v' L'S'M_L'M_S' \mid V_{kp} \mid d^n vLSM_LM_S) \\
&= \sum_{M_L(M_S)} \sum_{M_L'(M_S')} (LSM_LM_S \mid JM)(L'S'M_L'M_S' \mid J'M')(LkM_Lp \mid L'M_L') \\
&\qquad (d^n v' L'S' \| V_k \| d^n vLS) \\
&= (-1)^{L+k-L'} \sum_{M_L(M_S)} \sum_{M_L'(M_S')} (LSM_LM_S \mid JM)(L'S'M_L'M_S' \mid J'M') \\
&\qquad \times (kLpM_L \mid L'M_L')(d^n v' L'S' \| V_k \| d^n vLS) \\
&= (-1)^{L+k-L'} [(2L'+1)(2J+1)]^{1/2} W(kLJ'S'; L'J)(kJpM \mid J'M') \\
&\qquad \times (d^n v' L'S' \| V_k \| d^n vLS). \qquad (5)
\end{aligned}
$$

In this derivation, the Wigner–Eckart theorem and the following relationship between the Racah and Clebsch–Gordan coefficients are used[5]:

$$[(2e+1)(2f+1)]^{1/2} W(abcd; ef) C(afc; \alpha, \alpha+\delta) = \sum_\beta C(abe; \alpha\beta) C(edc; \alpha+\beta, \delta) C(bdf; \beta\delta), \qquad (6)$$

where

$$
\begin{aligned}
C(afc; \alpha, \beta+\delta) &\equiv (af\alpha\beta+\delta \mid c\alpha+\beta+\delta), \\
C(abe; \alpha\beta) &\equiv (ab\alpha\beta \mid e\alpha+\beta), \\
C(edc; \alpha+\beta, \delta) &\equiv (ed\alpha+\beta\delta \mid c\alpha+\beta+\delta), \\
C(bdf; \beta\delta) &\equiv (bd\beta\delta \mid f\beta+\delta),
\end{aligned}
$$

using the Condon and Shortley conventions.[6] The reduced matrix elements $(d^n v' L'S' \| V_k \| d^n vLS)$ in (5) can be calculated by means of a method based on the coefficients of fractional parentage. Explicit formulas are given by Brink and Satchler.[7]

As pointed out by Finkelstein and Van Vleck,[8] it is convenient to use as basis functions those which diagonalize the octahedral potential apart from elements nondiagonal in J. Such functions must be classified according to their cubic representation Γ rather than according to M. The transformation matrix $(J\Gamma \mid JM)$ can be found in Griffith's book[9] and is used here.

The matrix elements $(d^4 v' L'S'J'\Gamma_i \mid \mathcal{H}' \mid d^4 vLSJ\Gamma_i)$, $i = 1, \cdots, 5$, are thereby calculated and the nonvanishing ones are tabulated in Tables I to V. As seen from the tables, the crystalline-field matrix elements are given in terms of the parameter, Dq, where

$$q = (2/105) \langle r^4 \rangle. \qquad (7)$$

It is also necessary to note that the primed terms in Tables IV and V stem from the fact that these terms have two linearly independent Γ's of the same classification.

[5] M. E. Rose, *Elementary Theory of Angular Momentum* (John Wiley & Sons, Inc., New York, 1957), p. 110.
[6] E. V. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, Cambridge, England, 1953), p. 76.
[7] D. M. Brink and G. R. Satchler, *Angular Momentum* (Oxford University Press, London, 1962), p. 85.
[8] R. Finkelstein and J. H. Van Vleck, J. Chem. Phys. **8**, 790 (1940).
[9] J. S. Griffith, *The Theory of Transition Metal Ions* (Cambridge University Press, Cambridge, England, 1961), p. 393, Appendix 2, Table A19.