Calculation of Matrix Element of Electrostatic Interaction between p^4l and p^4l' for the Different Couplings

By

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Abstract

General formulae are given for the energy matrix of electrostatic interaction between configurations p^4l and p^4l' with $l' \neq l$. They are obtained for the Russell-Saunders coupling scheme as well as for the heterogeneous coupling scheme, in which one configuration is in the Russell-Saunders and the other in the pair coupling scheme. In both schemes, non-zero matrices are those with l' differing from l by 2. Present results are applicable to the calculation of the levels of singly ionized rare gas, in which the configuration interaction plays an important role.

Introduction

Since the advent of the rare gas laser, much attension is paid to the elementary parameters of rare gas atoms and ions. One is the electric dipole transition probability for spontaneous emission between the levels which have various configurations of singly ionized ions. The intermediate coupling calculation for rare gas ions was first performed by Garstang[1]. In order to get accurate eigenvector components of a level, various kinds of interaction between electrons should be taken into account. Especially it is often important to include the perturbation produced by interactions with other configurations. The singly ionized rare gas ions of the p^4l configuration with low l value ($l=0$, 1, 2) are well described by the Russell-Saunders coupling and those with high l value ($l=3$, 4) by the pair coupling[2]. The matrix elements of the electrostatic interaction operator between configurations with $l'=l$ in the Russell-Saunders coupling scheme were calculated by Yamanouchi et al.[3] and by Möller[4], those in the pair coupling scheme by Möller[4] and those in $J_c j$ coupling scheme by Minnhagen[5].

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In the present paper the configuration interactions between the p^4l and p^4l' configurations with $l' \neq l$ both in the Russell=Saunders and in the heterogeneous coupling schemes are given. The latter denotes one in the Russell-Saunders (LS) coupling and the other in the pair (JK) coupling.

The coupling of the core electrons

The p^4 configuration of the partially filled shell structure is the lowest lying energy state of doubly ionized rare gas ion. The electrons in this shell interact each other through the electrostatic and spin-orbit interactions. The complete transition from LS coupling to $J_c j$ coupling is plotted in Fig. 1. This is transcribed from Fig. 1[13] in TAS[6]. The curves show the relative intervals between the levels as a function of $\varkappa(\zeta/5F_2)$. The recently observed levels of Ne[7], Ar[8], Kr[9] and Xe[10] are also plotted in the figure in such a way that all the levels fit the theory as well as possible by the least-square method for each element. The parameter values $\varkappa$, F_2 and ζ of these levels are given in Table I. It is apparent from Fig. 1 and Table I that the coupling of the core electrons goes progressively from the LS to the $J_c j$ coupling as the atom gets heavier.

As for neon and argon, the cores are well described by the LS coupling scheme. While for kripton and xenon the cores are considerably apart from the LS coupling, then the mixing of level takes place. However, all the cores lie on the left half ($\varkappa < 1$)

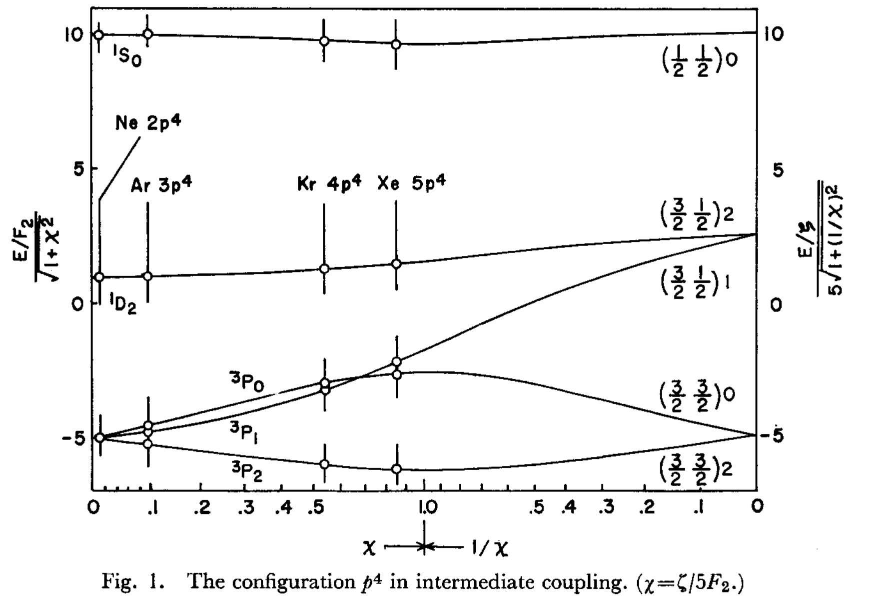

Fig. 1. The configuration p^4 in intermediate coupling. ($\chi = \zeta/5F_2$.)

Table I. Parameter values of χ, F_2 and ζ. ($\chi=\zeta/5F_2$.) They are determined to make the observed values best fit the theory by the least-square method.

	Ne	Ar	Kr	Xe
χ	0.01054	0.09513	0.5365	0.8473
F_2	3720	2178	1897	1784
ζ	196	1036	5089	7558

in Fig. 1, so that the coupling of the core is assumed to be described by the LS coupling in the present paper.

Electrostatic interaction for LS coupling scheme

It is well known from experimental study[2] that the configurations p^4l with $l=0$, 1, 2 can be well described by the aid of the LS coupling scheme, while those with $l=3$, 4 by the aid of the JK coupling scheme of Racah[11].

In order to get the matrix element of the electrostatic interaction, it is convenient to express the Coulomb interaction between electrons in tensor form[12]

$$\sum_{i>j} \frac{e^2}{r_{ij}} = e^2 \sum_{i>j} \sum_k \frac{r_<^k}{r_>^{k+1}} (\boldsymbol{c}_i^{(k)} \cdot \boldsymbol{c}_j^{(k)}) \,, \tag{1}$$

where $r_<$ is the lesser and $r_>$ the greater of r_i and r_j and $\boldsymbol{c}^{(k)}$ the tensor operator of rank k related to the usual spherical harmonics.

First we consider the case where both configurations of interest are in the LS coupling, that is,

$$p^4l \ : \ |\,(S_0, s)\, S, \quad (L_0, l)\, L, \ J> , \tag{2}$$

$$p^4l' \ : \ |\,(S_0, s)\, S', \quad (L_0', l')\, L', \ J> , \tag{2'}$$

where J is the total angular momentum of the state, S_0 and L_0 are the spin and orbital angular momentum of the p^4 core electrons, respectively, l is the orbital angular momentum of the running electron and S and L are the total spin and orbital angular momentum of the LS basis state, respectively. The matrix element for the LS coupling is expressed as follows:

$$<SLJ \left| \sum_{i>j} \frac{e^2}{r_{ij}} \right| S'L'J> = \sum_k \left[f_k\, R^k(n_0\, pnl,\, n_0\, pn'l') + g_k\, R^k(n_0\, pnl,\, n'l'\, n_0\, p) \right] \tag{3}$$

The Slater radial integral R^k is defined by

$$R^k(n_a\, l_a,\, n_b\, l_b;\, n_c\, l_c,\, n_d\, l_d) = e^2 \int_0^\infty \int_0^\infty \frac{r_<^k}{r_>^{k+1}} R_{n_a l_a}(r_1)\, R_{n_b l_b}(r_2) \times R_{n_c l_c}(r_1)\, R_{n_d l_d}(r_2)\, dr_1\, dr_2\,. \tag{4}$$

$R_{nl}(r)$ is the radial part of the hydrogenic wavefunction. The coefficients f_k and g_k are given after some computation as follows[13,14,15]:

$$f_k = \delta(S, S')\, \delta(L, L')\, \delta(S_0, S_0')\, (-1)^{L_0'+L+1} \cdot 3[l, l']^{1/2} \times \begin{pmatrix} 1 & k & 1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & k & l' \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} L & l & L \\ l' & L_0' & k \end{Bmatrix} (p^4\, \psi_0 \| U^{(k)} \| p^4\, \psi_0')\,, \tag{5}$$

$$g_k = \delta(S, S')\, \delta(L, L')\, (-1)^{S_0+S_0'} \cdot 12[l, l', S_0, L_0, S_0', L_0']^{1/2} \times \begin{pmatrix} l & k & 1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l' & k & 1 \\ 0 & 0 & 0 \end{pmatrix} \sum_{\bar{\psi}} (\psi_0\{|\bar{\psi})\, (\psi_0'\{|\bar{\psi}) \begin{Bmatrix} 1/2 & \bar{S} & S_0' \\ 1/2 & S & S_0 \end{Bmatrix} \begin{Bmatrix} \bar{L} & 1 & L_0' \\ 1 & k & l' \\ L_0 & l & L \end{Bmatrix}. \tag{6}$$

Here

$$[X, Y, \ldots\ldots] = (2X+1)\,(2Y+1)\ldots\ldots\,,$$

$$\begin{pmatrix} a & b & c \\ 0 & 0 & 0 \end{pmatrix} =:\ 3j - \text{coefficient},^{16)}$$

$$\begin{Bmatrix} a & b & c \\ d & e & f \end{Bmatrix} :\ 6j - \text{coefficient},^{16)}$$

$$\begin{Bmatrix} a & b & e \\ c & d & f \\ g & h & k \end{Bmatrix} :\ 9j - \text{coefficient},^{17)}$$

and $(\psi_0\{|\psi) = (S_0 L_0\{|SL)$ is the coefficient of fractional parentage[18] (CFP), and $(p^4\psi_0 \| U^{(k)} \| p^4\psi_0')$ is the matrix element of the tensor $U^{(k)}$, which is the sum of the unit tensors $u^{(k)}$ of the core.

The calculated results of f_k in eq. (5) and g_k in eq. (6) with $l' \neq l$ are given in Table II. This contains only those either of which is not trivial zero.

Electrostatic interaction for heterogeneous (LS-JK) coupling scheme

In order to estimate the coefiguration interaction between the configurations $p^4 l$ with $l=0, 1, 2$ and $p^4 l'$ with $l'=3, 4$, it is necessary to calculate the matrix element of the electrostatic interaction operator for the heterogeneous coupling scheme; one configuration is in the Russell-Saunders (LS) coupling scheme and the other in the pair (JK) coupling scheme, that is,

$$p^4l \quad : \quad |\,(S_0, s)\; S,\; (L_0, l)\; L, J> \,, \tag{7}$$

$$p^4l' \quad : \quad |\,((S_0', L_0')\; J_0, l')\; K, s, J> \,, \tag{7'}$$

where J_0 is the total angular momentum of the p^4 core electrons and K the intermediate angular momentum.

A state in JK coupling scheme may be expanded in terms of LS states as[19,20]

$$|\,((S_0', L_0')\; J_0, l')\; K, s, J> = \sum_{S,L} |\,(S_0', s)\; S, (L_0', l')\; L, J> U_{JK-LS'} \tag{8}$$

where

$$U_{JK-LS} = (-1)^{\,S_0'+L_0'+1/2+l'+S+L+2K}\,[J_0, K, S, L]^{1/2} \times \begin{Bmatrix} S & L & J \\ l' & K & L \end{Bmatrix} \begin{Bmatrix} L & S_0 & K \\ 1/2 & J & S \end{Bmatrix} . \tag{9}$$

Therefore, the matrix element to be worked out is obtained by using eqs. (8) and (9) in eq. (3) as

$$< SLJ\,|\sum_{i>j} \frac{e^2}{r_{ij}}\,|\,J_0KJ> = \sum_k (\tilde{f}_k R^k(pl, pl') + \tilde{g}_k R^k(pl, l'p)) \,, \tag{10}$$

where $\tilde{f}_k$ and $\tilde{g}_k$ are expressed as follows[19]:

$$\tilde{f}_k = (-1)^{S+S_0'+2K+l'+3/2} \cdot 3\,[l, l', S, L, J_0, K]^{1/2} \times \begin{pmatrix} 1 & k & k \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & k & l' \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} S_0' & L_0' & J_0 \\ l' & K & L \end{Bmatrix} \begin{Bmatrix} S & L & J \\ K & 1/2 & S_0' \end{Bmatrix} \begin{Bmatrix} L_0' & k & L_0 \\ l & L & l' \end{Bmatrix} \times (p^4 \psi_0 \,\|\, U^{(k)} \,\|\, p^4 \psi_0')\; \delta(S_0, S_0') \,, \tag{11}$$

$$\tilde{g}_k = (-1)^{S_0+S_0'} \cdot 12\,[l, l', S_0, L_0, S_0', L_0']^{1/2} \begin{pmatrix} l & k & 1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ l, & k & 1 \end{pmatrix} \times \sum (\psi_0\{|\bar{\psi})(\psi_0'\{|\bar{\psi}) \begin{Bmatrix} 1/2 & \bar{S} & S_0' \\ 1/2 & S & S_0 \end{Bmatrix} \begin{Bmatrix} \bar{L} & 1 & L_0' \\ 1 & k & l' \\ L & l & L \end{Bmatrix} . \tag{12}$$

The calculated results of $\tilde{f}_k$ and $\tilde{g}_k$ in eqs. (11) and (12) with $l' \neq l$ are given in Table III. Again in Table III, only the coefficients, either of which is not trivial zero, are listed.

Results and Discussion

The coefficients of the direct integral $\tilde{f}_k$ in eq. (5) and $\tilde{f}_k$ in eq. (11) contain two **3j**-coefficients. The first $3j$-coefficient is not zero only when k=0 or 2. The second

Table II. Coefficients f_k and g_k for the electrostatic integral $R^k(pl, pl')$ and $R^k(pl, l'p)$ in the Russell-Saunders coupling scheme with $l' \neq l$.

CORE	l	CORE	l'	S	L	f_2	$l=0$	g_{l+1}	g_1 (l=0)
${}^1S$	l	${}^1D$	$l+2$	1/2	l	$\frac{2\sqrt{3(l+1)(l+2)}}{5\sqrt{(2l+1)(2l+3)}}$	$\frac{2\sqrt{2}}{5}$	$-\frac{\sqrt{3(l+1)(l+2)}}{(2l+3)\sqrt{(2l+1)(2l+3)}}$	$-\frac{\sqrt{2}}{3}$
${}^1D$	l	${}^1S$	$l+2$	1/2	$l+2$	$\frac{2\sqrt{3(l+1)(l+2)}}{5\sqrt{(2l+3)(2l+5)}}$	$\frac{2\sqrt{10}}{25}$	$-\frac{\sqrt{3(l+1)(l+2)}}{(2l+3)\sqrt{(2l+3)(2l+5)}}$	$-\frac{\sqrt{10}}{15}$
${}^1D$	l	${}^1D$	$l+2$	1/2	$l+2$	$\frac{\sqrt{6(2l+7)(l+1)(l+3)}}{5(2l+3)\sqrt{2l+5}}$	$\frac{\sqrt{70}}{25}$	$-\frac{\sqrt{3(2l+7)(l+1)(l+3)}}{(2l+3)^2\sqrt{2(2l+5)}}$	$-\frac{\sqrt{70}}{30}$
					$l+1$	$\frac{3\sqrt{l(l+3)}}{5(2l+3)}$	0	$-\frac{3\sqrt{l(l+3)}}{2(2l+3)^2}$	0
					l	$\frac{(3l-2)\sqrt{6l(l+2)}}{5(2l+3)\sqrt{(2l-1)(2l+1)}}$	0	$-\frac{\sqrt{3(2l-1)l(l+2)}}{(2l+3)^2\sqrt{2(2l+1)}}$	0
${}^1D$	l	${}^3P$	$l+2$	1/2	$l+2$	0	0	$-\frac{3\sqrt{3(l+1)(l+3)}}{(2l+3)\sqrt{2(2l+3)(2l+5)}}$	$-\frac{\sqrt{30}}{10}$
					$l+1$	0	0	$-\frac{3\sqrt{3l(l+1)}}{2(2l+3)^2}$	0
${}^3P$	l	${}^1D$	$l+2$	1/2	$l+1$	0	0	$\frac{3\sqrt{3(l+2)(l+3)}}{2(2l+3)^2}$	$\frac{\sqrt{2}}{2}$
				1/2	l	0	0	$\frac{3\sqrt{3l(l+2)}}{(2l+3)\sqrt{2(2l+1)(2l+3)}}$	0
${}^3P$	l	${}^3P$	$l+2$	1/2	$l+1$	$-\frac{3\sqrt{(l+1)(l+2)}}{5(2l+3)}$	$-\frac{\sqrt{2}}{5}$	$\frac{9\sqrt{(l+1)(l+2)}}{2(2l+3)^2}$	$\frac{\sqrt{2}}{2}$
				3/2	$l+1$	$-\frac{3\sqrt{(l+1)(l+2)}}{5(2l+3)}$	$-\frac{\sqrt{2}}{5}$	0	0

Table III. Coefficients $\tilde{f}_k$ and $\tilde{g}_k$ for the electrostatic integral $R^k(pl, pl')$ and $R^k(pl, l'p)$ in the heterogeneous coupling scheme with $l' \neq l$.

CORE	S	L	CORE	J_0	K	J	$\tilde{f}_2$	$l=1$	$\tilde{g}_{l+1}$	$\tilde{g}_2\,(l=1)$
^1S	1/2	l	^1D	2	l	$l-1/2$	$-\frac{2\sqrt{3(l+1)(l+2)}}{5\sqrt{(2l+1)(2l+3)}}$	$-\frac{2\sqrt{30}}{25}$	$\frac{\sqrt{3(l+1)(l+2)}}{(2l+3)\sqrt{(2l+1)(2l+3)}}$	$\frac{\sqrt{30}}{25}$
				2	l	$l+1/2$	+ "	+ "	− "	− "
^3P	1/2	$l+1$	^3P	1	$l+1$	$l+1/2$	$\frac{\sqrt{6(l+1)(l+2)}}{10(2l+3)}$	$\frac{3}{25}$	$-\frac{3\sqrt{6(l+1)(l+2)}}{2^2(2l+3)^2}$	$-\frac{9}{50}$
				2	l		$-\frac{\sqrt{3(2l+1)(l+2)}}{5(2l+3)}$	$-\frac{3\sqrt{3}}{25}$	$\frac{3\sqrt{3(2l+1)(l+2)}}{2(2l+3)^2}$	$\frac{9\sqrt{3}}{50}$
				2	$l+1$		$-\frac{\sqrt{6(l+2)(l+3)}}{10(2l+3)}$	$-\frac{3\sqrt{2}}{25}$	$\frac{3\sqrt{6(l+2)(l+3)}}{2^2(2l+3)^2}$	$\frac{9\sqrt{2}}{50}$
				0	$l+2$	$l+3/2$	$-\frac{\sqrt{l+1}}{5\sqrt{2l+3}}$	$-\frac{\sqrt{10}}{25}$	$\frac{3\sqrt{(2l+3)(l+1)}}{2(2l+3)^2}$	$\frac{3\sqrt{10}}{50}$
				1	$l+1$		$\frac{(l+1)\sqrt{6(l+1)}}{10(2l+3)\sqrt{l+2}}$	$\frac{2}{25}$	$-\frac{3(l+1)\sqrt{6(l+1)}}{2^2(2l+3)^2\sqrt{l+2}}$	$-\frac{3}{25}$
				1	$l+2$		$\frac{\sqrt{6(l+1)(l+3)}}{10\sqrt{(2l+3)(l+2)}}$	$\frac{2\sqrt{5}}{25}$	$-\frac{3\sqrt{6(l+1)(l+3)}}{2^2(2l+3)\sqrt{(2l+3)(l+2)}}$	$-\frac{3\sqrt{5}}{25}$
				2	$l+1$		$-\frac{(l+1)\sqrt{6(l+3)}}{10(2l+3)\sqrt{l+2}}$	$-\frac{2\sqrt{2}}{25}$	$\frac{3(l+1)\sqrt{6(l+3)}}{2^2(2l+3)^2\sqrt{l+2}}$	$\frac{3\sqrt{2}}{25}$
				2	$l+2$		$-\frac{\sqrt{2(2l+7)(l+1)(l+3)}}{10(2l+3)\sqrt{l+2}}$	$-\frac{2\sqrt{3}}{25}$	$\frac{3\sqrt{2(2l+7)(l+1)(l+3)}}{2^2(2l+3)^2\sqrt{l+2}}$	$\frac{3\sqrt{3}}{25}$
^3P	1/2	l	^1D	2	l	$l-1/2$	0	0	$-\frac{3\sqrt{6l(l+2)}}{2(2l+3)\sqrt{(2l+1)(2l+3)}}$	$-\frac{3\sqrt{30}}{50}$

Table III. (Continued)

CORE	S	L	CORE	J_0	K	J	$\tilde{f}_2$	$l=1$	$\tilde{g}_{l+1}$	$\tilde{g}_2(l=1)$
				2	l	$l+1/2$	0	0	$\frac{3\sqrt{6l(l+2)}}{2(2l+3)\sqrt{(2l+1)(2l+3)}}$	$\frac{3\sqrt{30}}{50}$
^{3}P	1/2	$l+1$	^{1}D	2	$l+1$	$l+1/2$	0	0	$-\frac{3\sqrt{3(l+2)(l+3)}}{2(2l+3)^2}$	$-\frac{9}{25}$
				2	$l+1$	$l+3/2$	0	0	+ "	+ "
^{1}D	1/2	$l+2$	^{1}S	0	$l+2$	$l+3/2$	$-\frac{2\sqrt{3(l+1)(l+2)}}{5\sqrt{(2l+3)(2l+5)}}$	$-\frac{6\sqrt{70}}{175}$	$\frac{\sqrt{3(l+1)(l+2)}}{(2l+3)\sqrt{(2l+3)(2l+5)}}$	$\frac{3\sqrt{70}}{175}$
				0	$l+2$	$l+5/2$	+ "	+ "	− "	− "
^{1}D	1/2	$l+1$	^{3}P	1	$l+1$	$l+1/2$	0	0	$\frac{3\sqrt{2l(l+1)}}{2^2(2l+3)^2}$	$\frac{3}{50}$
				2	l		0	0	$-\frac{3\sqrt{(2l+1)l}}{2(2l+3)^2}$	$-\frac{3\sqrt{3}}{50}$
				2	$l+1$		0	0	$-\frac{3\sqrt{2l(l+3)}}{2^2(2l+3)^2}$	$-\frac{3\sqrt{2}}{50}$
				0	$l+2$	$l+3/2$	0	0	$-\frac{\sqrt{3l(l+1)}}{2(2l+3)\sqrt{(2l+3)(l+2)}}$	$-\frac{\sqrt{10}}{50}$
				1	$l+1$		0	0	$\frac{3(l+1)\sqrt{2l(l+1)}}{2^2(2l+3)^2(l+2)}$	$\frac{1}{25}$
				1	$l+2$		0	0	$\frac{3\sqrt{2l(l+1)(l+3)}}{2^2(2l+3)(l+2)\sqrt{2l+3}}$	$\frac{\sqrt{5}}{25}$
				2	$l+1$		0	0	$-\frac{3(l+1)\sqrt{2l(l+3)}}{2^2(2l+3)^2(l+2)}$	$-\frac{\sqrt{2}}{25}$

Table III. (Continued)

CORE	S	L	CORE	J_0	K	J	$\tilde{f}_2$	$l=1$	$\tilde{g}_{l+1}$	$\tilde{g}_2\,(l=1)$
				2	$l+2$		0	0	$-\frac{\sqrt{6(2l+7)l(l+1)(l+3)}}{2^2(2l+3)^2(l+2)}$	$-\frac{\sqrt{3}}{25}$
^1D	1/2	$l+2$	^3P	0	$l+2$	$l+3/2$	0	0	$\frac{(l+3)\sqrt{6(l+1)}}{2(2l+3)\sqrt{(2l+3)(2l+5)(l+2)}}$	$\frac{4\sqrt{35}}{175}$
				1	$l+1$		0	0	$-\frac{3(l+3)\sqrt{l+1}}{2(2l+3)(l+2)\sqrt{2l+5}}$	$-\frac{2\sqrt{14}}{35}$
				1	$l+2$		0	0	$-\frac{3\sqrt{(l+1)(l+3)}}{2(2l+3)(l+2)\sqrt{(2l+3)(2l+5)}}$	$-\frac{\sqrt{70}}{175}$
				2	$l+1$		0	0	$-\frac{3(l+1)\sqrt{l+3}}{2(2l+3)(l+2)\sqrt{2l+5}}$	$-\frac{2\sqrt{7}}{35}$
				2	$l+2$		0	0	$-\frac{\sqrt{3(2l+7)(l+1)(l+3)}}{2(2l+3)(l+2)\sqrt{2l+5}}$	$-\frac{\sqrt{42}}{35}$
				0	$l+2$	$l+5/2$	0	0	$\frac{\sqrt{6(l+1)(l+2)}}{2(2l+3)\sqrt{(2l+3)(2l+5)}}$	$\frac{3\sqrt{35}}{175}$
				1	$l+2$		0	0	$-\frac{3\sqrt{l+1}}{2(2l+3)\sqrt{(2l+3)(2l+5)(l+3)}}$	$-\frac{3\sqrt{70}}{700}$
				1	$l+3$		0	0	$\frac{3\sqrt{(2l+7)(l+1)(l+2)}}{2(2l+3)\sqrt{(2l+3)(2l+5)(l+3)}}$	$\frac{9\sqrt{210}}{700}$
				2	$l+2$		0	0	$-\frac{\sqrt{3(2l+7)(l+1)}}{2(2l+3)\sqrt{(2l+5)(l+3)}}$	$-\frac{3\sqrt{42}}{140}$
				2	$l+3$		0	0	$-\frac{3\sqrt{(2l+7)(l+1)(l+4)}}{2(2l+3)\sqrt{(2l+3)(2l+5)(l+3)}}$	$-\frac{9\sqrt{14}}{140}$

Table III. (Continued)

CORE	S	L	CORE	J_0	K	J	$\tilde{f}_2$	$l=1$	$\tilde{g}_{l+1}$	$\tilde{g}_2\,(l=1)$
^{1}D	1/2	l	^{1}D	2	l	$l-1/2$	$-\frac{(3l-2)\sqrt{6l(l+2)}}{5(2l+3)\sqrt{(2l-1)(2l+1)}}$	$-\frac{\sqrt{6}}{25}$	$\frac{\sqrt{6(2l-1)l(l+2)}}{2(2l+3)^2\sqrt{2l+1}}$	$\frac{\sqrt{6}}{50}$
				2	l	$l+1/2$	+ "	+ "	− "	− "
^{1}D	1/2	$l+1$	^{1}D	2	$l+1$	$l+1/2$	$-\frac{3\sqrt{l(l+3)}}{5(2l+3)}$	$-\frac{6}{25}$	$\frac{3\sqrt{l(l+3)}}{2(2l+3)^2}$	$\frac{3}{25}$
				2	$l+1$	$l+3/2$	+ "	+ "	− "	− "
^{1}D	1/2	$l+2$	^{1}D	2	$l+2$	$l+3/2$	$-\frac{\sqrt{6(2l+7)(l+1)(l+3)}}{5(2l+3)\sqrt{2l+5}}$	$-\frac{12\sqrt{21}}{175}$	$\frac{\sqrt{6(2l+7)(l+1)(l+3)}}{2(2l+3)^2\sqrt{2l+5}}$	$\frac{6\sqrt{21}}{175}$
				2	$l+2$	$l+5/2$	+ "	+ "	− "	− "
^{3}P	3/2	$l+1$	^{3}P	2	l	$l-1/2$	$\frac{3\sqrt{(l+1)(l+2)}}{5(2l+3)}$	$\frac{3\sqrt{6}}{25}$	0	0
				2	l	$l+1/2$	$-\frac{\sqrt{3}\,(l+2)}{5(2l+3)}$	$-\frac{3\sqrt{3}}{25}$	0	0
				1	$l+1$	$l+1/2$	$-\frac{\sqrt{6(2l+1)(l+1)}}{10(2l+3)}$	$-\frac{3}{25}$	0	0
				2	$l+1$	$l+1/2$	$-\frac{\sqrt{6(2l+1)(l+3)}}{10(2l+3)}$	$-\frac{3\sqrt{2}}{25}$	0	0
				0	$l+2$	$l+3/2$	$\frac{l+1}{5\sqrt{(2l+3)(2l+5)}}$	$\frac{2\sqrt{35}}{175}$	0	0
				1	$l+1$		$\frac{(l+1)\sqrt{6(2l+5)}}{10(2l+3)\sqrt{l+2}}$	$\frac{\sqrt{14}}{25}$	0	0

Table III. (Continued)

CORE	S	L	CORE	J_0	K	J	$\tilde{f}_2$	$l=1$	$\tilde{g}_{l+1}$	$\tilde{g}_2(l=1)$
				1	$l+2$		$-\frac{(l+1)\sqrt{6(l+3)}}{10\sqrt{(2l+3)(2l+5)(l+2)}}$	$-\frac{2\sqrt{7}}{175}$	0	0
				2	$l+1$		$-\frac{\sqrt{6(2l+5)(l+1)(l+3)}}{10(2l+3)\sqrt{l+2}}$	$-\frac{2\sqrt{7}}{25}$	0	0
				2	$l+2$		$\frac{(l+1)\sqrt{2(2l+7)(l+3)}}{10(2l+3)\sqrt{(2l+5)(l+2)}}$	$\frac{2\sqrt{42}}{175}$	0	0
				0	$l+2$	$l+5/2$	$-\frac{\sqrt{3(l+1)(l+2)}}{5\sqrt{(2l+3)(2l+5)}}$	$-\frac{3\sqrt{70}}{175}$	0	0
				1	$l+2$		$\frac{3\sqrt{2(l+1)(l+3)}}{10\sqrt{(2l+3)(2l+5)}}$	$\frac{6\sqrt{35}}{175}$	0	0
				2	$l+2$		$-\frac{\sqrt{6(2l+7)(l+1)(l+3)}}{10(2l+3)\sqrt{2l+5}}$	$-\frac{6\sqrt{21}}{175}$	0	0

shows that $|l'-l|=2$ for $k=2$ when $l' \neq l$. Then the coefficients f_2 and $\tilde{f}_2$ remain non-zero.

The coefficients of the exchange integral g_k in eq. (6) and g_k in eq. (12) contain two $3j$-coefficients, too. In the same way as above, the coefficients g_{l+1} and g_{l+1} are non-zero.

In Tables II and III, all the coefficients are given as a function of l and the corresponding numerical values for $l=0$ and 1 are also given. The coefficients with $l=0$ are applied to the estimation of the configuration interaction between p^4s and p^4d in LS coupling scheme. On the other hand, those with $l=1$ are applied to estimate the configuration interaction between p^4p in LS and p^4f in JK coupling schemes.

The coefficients f_k and g_k with $l'=l$ using eqs. (5) and (6) coincide with those obtained by Yamanouchi et al[3].

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