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Checks of the Algebraic Matrices for the Configurations $(d+s)^n p$*

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By constructing suitable combinations of algebraic matrices enabling the resulting eigenvalues to be predicted theoretically, checking parameters were obtained for 32 interaction parameters of the configuration $(d+s)^n p$.

Key words: Checking parameters; $(d+s)^n p$; electrostatic interaction; relative phases; spin-orbit interaction.

1. Introduction

The algebraic matrices of $(d+s)^n p$ comprise the electrostatic and spin-orbit interaction matrices of the configurations $d^n p$, $d^{n-1}sp$ and $d^{n-2}s^2p$, the matrices of the correction parameters representing two and three body interactions of the core d electrons, as well as the interactions between configurations. The energy matrix (for a particular n) is then a linear combination of these matrices, the coefficients of which are parameters usually obtained empirically by fitting the experimental levels to the eigenvalues of the energy matrix. In a previous paper, [1][1], the role and significance of the various parameters was discussed.

The algebraic matrices of $(d+s)^n p$ were constructed and checked by the author with the purpose of using them to explain and predict the spectra of the configurations $(3d+4s)^n 4p$ in neutral and singly-ionized atoms of the iron group. The problem of constructing the matrices was considered previously [2-4]. By using the eigenvalues of the Casimir operator for the group SU_3, checking parameters were obtained for 12 electrostatic interaction matrices of the configuration $(d+s)^n p$, [1]. The purpose of the present paper is to obtain checking parameters for the remaining interaction parameters. The checked matrices of the configurations $(d+s)^n p$, for all permissible n, are available and can be obtained by request.

All checks are based upon the construction of such algebraic matrices so that the eigenvalues of the resulting matrix may be predicted theoretically. If we know the values of the parameters required in order to form the desired combinations, then we insert these values as coefficients multiplying the algebraic matrices found on tape, and diagonalize the resulting matrix. If the obtained eigenvalues differ from those predicted theoretically then it is usually not too difficult to find the reason for the discrepancy because in a particular check only a few of the parameters are utilized.

2. The Check ^1P

In this check we do not obtain exact numerical values of the predicted eigenvalues, only the number of eigenvalues differing from zero in any particular term of $(d+s)^n p$. We first choose the

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[1] Figures in brackets indicate the literature references at the end of this paper.

parameters of the configurations $(d+s)p$ in such a way that as many terms as possible of $(d+s)p$ should have vanishing eigenvalues. By adding two parameters to the electrostatic parameters of $(d+s)p$, it is found that we can cause all the eigenvalues of $(d+s)p$, except one, to equal zero. Since the configuration $(d+s)^n p$ can be obtained from $(d+s)p+(d+s)^{n-1}$, it is most convenient to choose the nonvanishing term of $(d+s)p$ with lowest L and S, i.e., ^{1}P. If, furthermore, the rank of the 2×2 matrix of ^{1}P in $(d+s)p$ is equal to 1, then when considering a particular term of $(d+s)^n p$, the rank of its matrix equals the number of terms of $(d+s)^{n-1}$, which in combination with ^{1}P yield the desired term of $(d+s)^n p$. By choosing ^{1}P of $(d+s)p$ to be nonvanishing the matrices of $(d+s)^n p$ are of the lowest rank and thus have a maximal number of vanishing eigenvalues.

In the configuration dp there are the six terms ^{1,3}PDF and in the configuration sp the two terms are ^{1,3}P. We may be inclined at first to search for parameters which would cause all the terms of $(d+s)p$ to vanish identically. However, for this purpose we need 11 parameters to solve the resulting 10 homogeneous equations, whereas the number of electrostatic parameters of $(d+s)p$ is only 8, i.e., F_0,F_2, G_1,G_3, F_0', G'_{ps}, J and K. It is, however, possible to add two additional parameters which are independent of the previous six. We thus add to each term of $(d+s)p$

$$\epsilon\,(l_1\cdot l_2)+\mu(\mathrm{s}_1\cdot \mathrm{s}_2).$$

For d-p this contribution equals

$$\begin{aligned}&\epsilon/2\,[L(L+1)-l_d(l_d+1)-l_p(l_p+1)]\\&+\mu/2\,[S(S+1)-s_d(s_d+1)-s_p(s_p+1)]\\&=\epsilon/2\,[L(L+1)-8]+\mu/2\,[S(S+1)-3/2].\end{aligned}\tag{1}$$

For $s-p$ we have

$$\begin{aligned}\epsilon/2\,[L(L+1)-l_s(l_s+1)-l_p(l_p+1)]+\mu/2\,[S(S+1)-s_s(s_s+1)-s_p(s_p+1)]\\=\mu/2\,[S(S+1)-3/2].\end{aligned}\tag{2}$$

Here L and S are the net angular momentum and spin respectively, of a particular term of $(d+s)p$. We note that here the definitions of ϵ and μ differ slightly from those of the parameters λ and δ introduced in a previous paper, [1].

From p. 200 TAS [5], and (1) the terms of dp can be written as

$$\begin{aligned}{}^1\mathrm{P}&=F_0+7F_2+G_1+21G_3-3\epsilon-3/4\,\mu\\{}^3\mathrm{P}&=F_0+7F_2-G_1-21G_3-3\epsilon-1/4\,\mu\\{}^1\mathrm{D}&=F_0-7F_2-3G_1+7G_3-\epsilon-3/4\,\mu\\{}^3\mathrm{D}&=F_0-7F_2+3G_1-7G_3-\epsilon+1/4\,\mu\\{}^1\mathrm{F}&=F_0+2F_2+6G_1+G_3+2\epsilon-3/4\,\mu\\{}^3\mathrm{F}&=F_0+2F_2-6G_1-G_3+2\epsilon+1/4\,\mu\,.\end{aligned}\tag{3}$$

The two terms of sp are

$$\begin{aligned}{}^1\mathrm{P}'&=F_0'+G'_{ps}-3/4\,\mu\\{}^3\mathrm{P}'&=F_0'-G'_{ps}+1/4\,\mu\,.\end{aligned}\tag{4}$$

In (3) we have six equations with six independent parameters. Thus, we can let five of the equations to equal zero and the sixth to differ from zero. As stated previously, the term chosen to differ from zero is ^{1}P. On solving (3) we obtain parameters proportional to the following:

$$F_0=35, F_2=5, G_1=4, G_3=6, \epsilon=-15 \text{ and } \mu=60\,.\tag{5}$$

The value of ^1P is then equal to 200.

For sp we require that $^3P'$ be equal to zero, and thus form (4) and (5)

$$\begin{aligned} {}^1P' &= F_0' + G'_{ps} + 45 \\ 0 &= F_0' - G'_{ps} + 15. \end{aligned} \tag{6}$$

The interaction between configurations dp and sp is given by equation (7), [4]. For ^1P this equals $-\sqrt{2}(J+K)$, whereas for ^3P the interaction equals $-\sqrt{2}(J-K)$. Furthermore, since the matrix of ^3P is to be identically equal to zero, the nondiagonal contribution also vanishes.

Thus

$$J = K. \tag{7}$$

The matrix of $(dp+sp)$ then reduces to the 2×2 matrix of ^1P which is given by

$$^1P = \begin{pmatrix} 200 & -2\sqrt{2}J \\ -2\sqrt{2}J & 2F_0' - 30 \end{pmatrix}. \tag{8}$$

For the above matrix to be of rank 1 its determinant must vanish. Then,

$$50\ F_0' - 750 = J^2. \tag{9}$$

We can choose

$$J = K = 10\sqrt{10}. \tag{10}$$

Then

$$F_0' = 35. \tag{11}$$

By (6)

$$G'_{ps} = 50. \tag{12}$$

Then by (5)

$$S' = F_0' - F_0 = 0. \tag{13}$$

With the choice of parameters given by (5), (10), (11), (12), and (13) the only nonvanishing eigenvalue of $(d+s)p$ is that of ^1P. By inserting the values of F_0' and J into (8) the numerical value of this eigenvalue is found to equal 240.

Instead of the matrices ϵ and μ we must use the matrices of α, λ, and δ since the latter are on tape for all $(d+s)^n p$. From the definitions of the parameters α, λ, and δ and noting that the core of $(d+\ )p$ is $(d+s)$, we have from p. 32 [1]

$$\begin{aligned} \lambda &= \epsilon/2 = -7.5 \\ \alpha &= -\epsilon/2 = 7.5 \\ \delta &= \mu/2 = 30. \end{aligned} \tag{14}$$

In addition there is a constant contribution $-\epsilon/2\ l_p(l_p+1) - \mu/2\ s_p(s_p+1) = -7.5$.

Thus, we must add -7.5 to the height of $(d+s)^n p$. Now, for dp

$$A = F_0(dp) = 35. \tag{15}$$

For $d^n p$ there are only n interactions $d-p$ as the parameters B and C of the interaction $d-d$ are set equal to zero in this check. Furthermore, taking into account the above contribution of -7.5 we have

$$A(d^n p) = 35n - 7.5. \tag{16}$$

Since in addition to the $d-d$ interaction, the $d-s$ interaction is also equal to zero, and $F_0'(ps)$ equals $F_0(dp)$, we have that the A's of the configurations $d^n p$ and $d^{n-1}sp$ are equal. Thus $S'(d^{n-1}sp)$ equals zero.

For $d^{n-2}s^2p$ we must take into account the constant $-G'_{ps}$ for each term, which is not put on tape.

Then we have

$$S''=-G'_{ps}=-50. \tag{17}$$

Thus, finally we have the following parameters for the check ${}^1P$ of the configuration $(d+s)^n p$:

$$\begin{aligned}
&A(d^n p) = 35n-7.5\\
&S' \quad\;\; =0\\
&S'' \quad\; =-50\\
&F_2=F_2'=F_2''=5\\
&G_1=G_1'=G_1''=4\\
&G_3=G_3'=G_3''=6\\
&G_{ps}' \quad =50\\
&\alpha=\alpha' \;=\alpha''=7.5\\
&J=J' \;=K=K'=10\sqrt{10}\\
&\lambda=\lambda' \;=\lambda''=-7.5\\
&\delta=\delta' \;=\delta''=30.
\end{aligned} \tag{18}$$

For the configuration $(d+s)^2p$, the matrices of α', λ'' and δ'' are constants and were thus not put on tape. However, we must take these parameters into account by incorporating them into S' and S''.

Thus,

$$S'(dsp)=0+6\times 7.5=45$$

$$S''(s^2p)=-50+3/4\times 30-2\times 7.5=-42.5. \tag{19}$$

In the configuration $(d+s)^3p$, the matrix of α'' is a constant and thus not on tape.

Therefore,

$$S''(ds^2p)=-50+6\times 7.5=-5. \tag{20}$$

It should be noted that in this check there is considerable freedom in choosing the checking parameters. Firstly, the parameters of (5) can be replaced by parameters whose values are proportional to those of (5). Also we can choose the values of F_0' and J in any convenient way as long as (9) is satisfied. Finally, it is not necessary to cause ${}^1P$ to be the only nonvanishing term. By the same token we can choose ${}^3P$ to be nonvanishing. The latter choice would only increase the rank of the matrix of a particular term of $(d+s)^n p$, which is obtained by the combination of $(d+s)^{n-1}+{}^3P$.

Since we have chosen the matrix of ${}^3P$ to be vanishing, J is equal to K in this check and thus nondiagonal elements of the interaction between configurations which are proportional to $(J-K)$ can be wrong and we would not notice this fact from the ${}^1P$ check. However, the matrices of J are checked independently in the Casimir Check [1], and thus if there is an error of the nature mentioned above we would detect it from the Casimir Check.

Since the ${}^1P$ Check includes the parameters G_1,G_3, K and K', whose matrices differ for complementary configurations [4], we may be inclined to use this check for $n>6$. However, in its present form the ^{1}P Check is useless for $n>6$. This follows from the fact that for $n>6$ the number of possibilities of combining $(d+s)^{n-1}$ with ^{1}P of $(d+s)p$ to yield a particular term of $(d+s)^n p$ is greater than the order of the matrix considered. Thus, the check ^{1}P for $(d+s)^n p$, where $n>6$, must be modified by choosing $(d+s)^{11}p$ as the basic configuration rather than $(d+s)p$. Now, $(d+s)^{11}p$ can be considered as $(d+s)^{-1}p$ by the notation of section 3, [4].

From p. 229 TAS, [5], it is evident that in order for all the terms except ^{1}P of d^9s^2p, i.e., $d^{-1}p$, to equal zero, we must have

$$F_0(d^{-1}p)=F_2=G_3=\epsilon=\mu=0. \tag{21}$$

$$G_1\neq 0. \tag{22}$$

Then,

$${}^1\mathrm{P}=20G_1. \tag{23}$$

For the terms of $d^{10}sp$, i.e., $s^{-1}p$, the interaction $s^{-1}-p$ is the same as the interaction $s-p$ and so we have

$${}^3\mathrm{P}'=F_0'(s^{-1}p)-G'_{ps}. \tag{24}$$

$${}^1\mathrm{P}'=F_0'(s^{-1}p)+G'_{ps}. \tag{25}$$

If, as before, we require that ^{3}P be equal to zero then

$$F_0'(s^{-1}p)=G'_{ps}. \tag{26}$$

$${}^1\mathrm{P}'=2F_0'(s^{-1}p). \tag{27}$$

The interaction between the configurations $d^{10}sp$ and d^9s^2p is given by (8), [4]. For ^{1}P this equals $\sqrt{2}(J'-2K')$ whereas for ^{3}P we have the value of $\sqrt{2}J'$ for this interaction. Since the matrix of the term ^{3}P must be equal to zero identically, we have

$$J'=0. \tag{28}$$

Then the matrix of ^{1}P can be written as

$${}^1\mathrm{P}=\begin{pmatrix} 20G_1 & -2\sqrt{2}K' \\ -2\sqrt{2}K' & 2G'_{ps} \end{pmatrix} \tag{29}$$

We specify that the above matrix be of rank 1, and thus its determinant must vanish. This implies

$$40G_1\,G'_{ps}=8(K')^2. \tag{30}$$

As before, we can let

$$G_1=4,\ G'_{ps}=50 \text{ and } K'=10\sqrt{10}. \tag{31}$$

Then,

$$F_0'(s^{-1}p)=G'_{ps}=50. \tag{32}$$

The single nonvanishing eigenvalue of the matrix (29) is then equal to 180.

For $(d+s)^{11}p$ the following parameters enter the ^{1}P Check:

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$$\begin{aligned}
A(d^9s^2p) &= A(d^{-1}p) = 0 \\
A'(d^{10}sp) &= A'(s^{-1}p) = 50 \\
S' &= 50 \\
G_1 &= 4 \\
G'_{ps} &= 50 \\
K' &= 10\sqrt{10}.
\end{aligned} \tag{33}$$

In order to obtain the parameters for $(d+s)^{12-n}p$ where $n<6$, we write $(d+s)^{12-n}p$ as $(d+s)^{-n}$, i.e., the configuration comprising n holes in the $(d+s)$ shells.

$$\begin{aligned}
A(d^{10-n}s^2p) &= A(d^{-n}p) = nA(d^{-1}p) = 0 \\
A'(d^{11-n}sp) &= A'(d^{-[n-1]}s^{-1}p) = A'(d^{-[n-1]}p) + A'(s^{-1}p) = 0 + 50 = 50 \\
A''(d^{12-n}p) &= A''(d^{-[n-2]}s^{-2}p) = A''(d^{-[n-2]}p) + 2A'(s^{-1}p) - G'_{sp} = 0 + 100 - 50 = 50.
\end{aligned} \tag{34}$$

Thus,

$$\begin{aligned}
A &= 0 \\
S' &= 50 \\
S'' &= 50 \\
G_1 &= 4 \\
G'_{ps} &= 50 \\
K &= K' = 10\sqrt{10}.
\end{aligned} \tag{35}$$

In this check we have the result that for a particular term of $(d+s)^{-n}p$, the rank of the matrix equals the number of terms of $(d+s)^{-(n-1)}$, which can be combined with ^{1}P to yield the particular terms of $(d+s)^{-n}p$. This result is exactly analogous to the previous result since the configuration $(d+s)^{-n}$ has exactly the same terms as $(d+s)^n$, and similarly for $(d+s)^np$ and $(d+s)^{-n}p$. Tables 1-4 give the ranks of the matrices for each term of $(d+s)^np$ (or equivalently for each term of $(d+s)^{-n}p$).

As an example, from table 3 the rank of the matrix of $(d+s)^5p\,^3$D, or equivalently $(d+s)^7p\,^3$D, is 13. From table 6, [1], the number of expected eigenvalues of ^{3}D is 29. Thus for the ^{1}P check of $(d+s)^5p$, with parameters given by (18) or for the ^{1}P check of $(d+s)^7p$, with parameters given by (32), the matrix of ^{3}D should yield 16 vanishing eigenvalues and 13 eigenvalues differing from zero. When the rank of a particular term is not specified, it is zero and thus all the eigenvalues of that term should vanish.

TABLE 1. *Predicted number of nonzero eigenvalues for* $(d+s)^{\pm 2}p$

Term	Rank
^{2}P	2
^{2}D	1
^{2}F	1

TABLE 2. *Predicted number of nonzero eigenvalues for* $(d + s)^{\pm 3}p$

Term	Rank
^1P	4
^1D	2
^1F	3
^1G	1
^1H	1
^3S	1
^3P	2
^3D	3
^3F	2
^3G	1

TABLE 3. *Predicted number of nonzero eigenvalues for* $(d + s)^{\pm 4}p$

Term	Rank
^2S	2
^2P	7
^2D	8
^2F	8
^2G	5
^2H	3
^2I	1
^4S	2
^4P	2
^4D	4
^4F	2
^4G	2

TABLE 4. *Predicted number of nonzero eigenvalues for* $(d + s)^{\pm 5}p$

Term	Rank
^1S	1
^1P	9
^1D	8
^1F	11
^1G	7
^1H	6
^1I	2
^1K	1
^3S	5
^3P	8
^3D	13
^3F	10
^3G	9
^3H	4
^3I	2
^5S	1
^5P	2
^5D	3
^5F	2
^5G	1

TABLE 5. *Predicted number of nonzero eigenvalues of* $(\mathrm{d}+\mathrm{s})^6\mathrm{p}$

Term	Rank
$^2\mathrm{S}$	4
$^2\mathrm{P}$	15
$^2\mathrm{D}$	18
$^2\mathrm{F}$	20
$^2\mathrm{G}$	15
$^2\mathrm{H}$	11
$^2\mathrm{I}$	5
$^2\mathrm{K}$	2
$^4\mathrm{S}$	4
$^4\mathrm{P}$	7
$^4\mathrm{D}$	11
$^4\mathrm{F}$	9
$^4\mathrm{G}$	7
$^4\mathrm{H}$	3
$^4\mathrm{I}$	1
$^6\mathrm{P}$	2
$^6\mathrm{D}$	1
$^6\mathrm{F}$	1

3. The Check Delta

With the aid of the modified $^1\mathrm{P}$ Check for $(d+s)^{12-n}p$, where $n<6$, it was possible to check the matrices of G_1,[2] K and K'. However, it is still necessary to check the matrices of G_3 for these configurations. By means of the Check Delta we obtain checks of the matrices of G_1 and G_3 for $(d+s)^{12-n}p$, where $n<6$, as well as for the matrices of F_2, G_1 and G_3 for the complementary configurations of $(d+s)^{12-n}p$, i.e., $(d+s)^n p$.

If we insert for the configuration dp, the values

$$F^k = G^k = (2k+1)F^0, \tag{36}$$

which are the values corresponding to a δ-interaction [6], we get nonvanishing eigenvalues only for $^1\mathrm{P}$ and $^1\mathrm{F}$. If in addition we give G^k the value

$$G^k = -(2k+1)F^0, \tag{37}$$

the resulting matrices of $dp + d^9p$ vanish identically, [7] and [8].

Now, from the definitions of the parameters F_1, G_1 and G_3 [1]

$$F_0 = F^0 = 35 \tag{38}$$

we obtain

$$F_2 = 5,\ G_1 = 7,\ G_3 = 3,\ \mathrm{G}_1 = -7,\ \mathrm{G}_3 = -3. \tag{39}$$

For the configurations d^np and $d^{10-n}s^2p$, the height A is given by

$$A = nF_0 = 35n \tag{40}$$

as only the $d-p$ interaction is taken into account in this check.

Similarly for the configurations $d^{n-1}sp$ and $d^{11-n}sp$ as well as $d^{n-2}s^2p$ and $d^{12-n}p$ we have

[2] (G_1 and G_3 are the parameters of $(d+s)^{12-n}p$, where $n<6$, to distinguish from G_1 and G_3 of $(d+s)^np$, which are on the same tape.)

$$
\begin{aligned}
A' &= (n-1)F_0 = 35(n-1) \\
A'' &= (n-2)F_0 = 35(n-2) \\
S' &\qquad\quad = -35 \\
S'' &\qquad\quad = -70.
\end{aligned}
\tag{41}
$$

The other parameters are given by (38), (39) and (40).

This check is useful, simple and very convenient as all the expected eigenvalues vanish. The Check Delta may be particularly helpful in the case where by chance the other checks may not locate the error.

4. The Check C, G'_{ds} and β

The primary purpose of this check is to verify that the matrices of C and β are correct. Incidentally, the matrices of G'_{ds} and δ are also checked. In our case δ has no physical significance since it is only a checking parameter, [1]. Since only the parameters C, G'_{ds}, β and δ enter this check, it is used for $n \leqslant 6$.

From (88′) [9], the energy of d^n, for the case of B equal to zero, is given by

$$W = \sum_{i<j} W_{ij} = \sum_{i<j} [A + \tfrac{1}{2} - \{2(\mathrm{s}_i \cdot \mathrm{s}_j) + q_{ij}\}C]$$

Here s_i and s_j are spins of the electrons i and j, and $\sum_{i<j} q_{ij}$ is the seniority operator Q((50), [10]). By (91) [9],

$$2\sum_{i<j} (\mathrm{s}_1 \cdot \mathrm{s}_j) = S_1(S_1+1) - \tfrac{3}{4}\, n,$$

where S_1 is the net spin of d^n.

Since there are $n(n-1)$ pairs in the summation we have

$$W = \frac{n(n-1)}{2} A + \left[\frac{n(n+2)}{4} - S_1(S_1+1) + Q\right] C. \tag{42}$$

Since $\dfrac{n(n-1)}{2}$ is a constant for a particular d^np under consideration, we can replace A by $\dfrac{n(n-1)}{2} A$ as the height of the configuration, and call the result simply A. To (42) we add βQ and $\delta[S(S+1) - S_1(S_1+1)]$, where S is the spin of d^np.

Then, (42) becomes

$$W = A + \left[\frac{n(n+2)}{4} - S_1(S_1+1) + Q\right] C + \beta Q + \delta[S(S+1) - S_1(S_1+1)]\,. \tag{43}$$

If we now let

$$C = -4,\ \beta = 4 \text{ and } \delta = 4, \tag{44}$$

we get

$$W = A - n(n+2) + 4S(S+1). \tag{45}$$

If, furthermore, all the other parameters of d^np are given a value equal to zero and

$$A = (n+1)^2 \tag{46}$$

we have the very simple result

$$W(d^n p) = (2S+1)^2. \tag{47}$$

For the configurations $d^{n-1}sp$ we let S, S_2 and S_1 be the net spins of $d^{n-1}sp$, $d^{n-1}s$ and d^{n-1}, respectively. Then from (43) we obtain

$$W(d^{n-1}sp) = A' + \left[\frac{(n-1)(n+1)}{4} - S_1(S_1+1) + Q'\right]C' + \beta' Q' + \delta'[S(S+1) - S_2(S_2+1)]. \tag{48}$$

By using the parameters for C', β' and δ' as given in (44) we get

$$W(d^{n-1}sp) = A' - n^2 + 1 + 4S_1(S_1+1) - 4S_2(S_2+1) + 4S(S+1). \tag{49}$$

The term $S_1(S_1+1) - S_2(S_2+1)$ can be compensated for by the coefficient of G'_{ds} which by (32), [2] equals

$$-\tfrac{1}{2}[(n-1) + 4\mathrm{S}_1 \cdot \mathrm{s}] = -\frac{(n-1)}{2} - S_2(S_2+1) + S_1(S_1+1) + \tfrac{3}{4}. \tag{50}$$

Then, by giving G'_{ds} a value equal to -4 we obtain from (49) and (50)

$$W(d^{n-1}sp) = A' - n^2 + 2n - 4 + 4S(S+1). \tag{51}$$

Then letting

$$A' = n^2 - 2n + 5, \tag{52}$$

we have

$$W(d^{n-1}sp) = (2S+1)^2. \tag{53}$$

From (46) and (52)

$$S' = A' - A = -4(n-1). \tag{54}$$

From (43),

$$W(d^{n-2}s^2p) = A'' + \left[\frac{n(n-2)}{4} - S_1(S_1+1) + Q''\right]C'' + \beta'' Q'' + \delta''[S(S+1) - S_1(S_1+1)]. \tag{55}$$

Here S, S_1 are the spins of $d^{n-2}s^2p$ and d^{n-2} respectively, and A'' includes the $d-s$ interaction of $d^{n-2}s^2p$, which is a constant, [4].

We let

$$\beta'' = 4,\ C'' = -4,\ \delta'' = 4.$$

Then,

$$W(d^{n-2}s^2p) = A'' - n(n-2) + 4S(S+1). \tag{56}$$

Thus, if we let

$$A'' = (n-1)^2, \tag{57}$$

then

$$W(d^{n-2}s^2p) = (2S+1)^2. \tag{58}$$

From (46) and (57) we have

$$S'' = A'' - A = -4n. \tag{59}$$

Thus, the following parameters are used in this check:

$$\begin{aligned} A &= (n+1)^2 \\ S' &= -4(n-1) \\ S'' &= -4n \\ C &= C' = C'' = -4 \\ G'_{ds} &= -4 \\ \beta &= \beta' = \beta'' = 4 \\ \delta &= \delta' = \delta'' = 4\,. \end{aligned} \tag{60}$$

The expected eigenvalues then equal $(2S+1)^2$, where S is the net spin of the term considered in either $d^n p$, $d^{n-1}sp$ or $d^{n-2}s^2p$.

For $(d+s)^6p$ we must be particularly careful to modify the heights. Since the matrices of C, β, and δ are the same for d^6p as for d^4s^2p we have here

$$W(d^6p) = W(d^4s^2p). \tag{61}$$

However, from (57)

$$A''(d^4s^2p) = 25.$$

Thus,

$$A(d^6p) = 25.$$

Also, from (52)

$$A'(d^5sp) = 29.$$

Thus, the heights of $(d+s)^6p$ are given by

$$\begin{aligned} A(d^6p) &= 25 \\ S' &= 4 \\ S'' &= 0\,. \end{aligned} \tag{62}$$

In the configuration $(d+s)^2p$, the coefficient of δ'' is a constant. Since the matrix of δ'' is not put on tape, it must be incorporated into S''.

For s^2p,

$$S(S+1) - S_1(S_1+1) = 3/4.$$

Then,

$$S''(s^2p) = -8 + (3/4)(4) = -5.$$

5. The Check T and T_c

The configurations d^n for $n < 5$ are characterized by the parameter T [1], whereas the configurations d^n for $n > 5$ are characterized by T_c [2]. The configuration d^5 can be considered as either consisting of 5 electrons d or as 5 holes in the d shell. In the former case the parameter needed is T, whereas in the latter case the parameter T_c is to be used. The relationship between these two cases is given by (65), [10].

An interesting and very useful relationship was obtained by Racah [11] for the configuration d^n. If we let

$$\begin{aligned} C &= -80 \\ \alpha &= 15 \\ \beta &= 160 \\ T &= 1 \\ T_c &= 1 \end{aligned} \tag{63}$$

then,

$$W(d^n) = 240 - 40(n-2)(n-3). \tag{64}$$

Since the matrices of T and T_c for the configurations $d^n p$, $d^{n-1}sp$ and $d^{n-2}s^2p$ are just those of d^n, d^{n-1} and d^{n-2}, the equations (63) and (64) can be used to check the matrices of these parameters in the configurations $(d+s)^n p$. It should be noted that although T and T_c are parameters representing three-body interactions, [1], the combination $T+T_c$ represents two-body interactions, the same as the interactions represented by C, α, and β, [1].

Incidentally, the matrices of C, α, and β are checked here. However, as they enter other checks as well, the primary purpose here is to verify that the matrices of T and T_c are correct.

6. The Checks of the Spin-Orbit Interaction Matrices

In order to check the matrices of either ζ_d or ζ_p it is sufficient to diagonalize them separately giving a value of zero to all the other parameters. The expected eigenvalues may be obtained by determining the possible states of the configuration considered in $j-j$ coupling.

Since for an electron d, j can take on the values 3/2 or 5/2

$$\begin{aligned} (\mathbf{l}\cdot\mathbf{s}) &= \tfrac{1}{2}\,[j(j+1) - l(l+1) - s(s+1)] \\ &= 1, \text{ for } d_{5/2} \\ &= -\tfrac{3}{2}, \text{ for } d_{3/2}. \end{aligned} \tag{65}$$

The eigenvalues for d^n are then obtained by determining the combinations of $d_{3/2}$ and $d_{5/2}$ making up d^n.

For an electron p, j has the values 1/2 and 3/2.

Thus,

$$\begin{aligned} (\mathbf{l}\cdot\mathbf{s}) &= \tfrac{1}{2}, \text{ for } p_{3/2} \\ &= -1, \text{ for } p_{1/2}. \end{aligned} \tag{66}$$

In order to determine the multiplicity of each eigenvalue for a particular J, it is necessary to know what multiplicities of J appear in the configuration $[d_{5/2}]^k\,[d_{3/2}]^{n-k}$. The resulting J of $[d_{5/2}]^k$ and $[d_{3/2}]^{n-k}$, with their respective multiplicities are given on p. 263, TAS [5]. By using this information it is easy to obtain the multiplicities of the eigenvalues of the matrix ζ_d in the configuration d^n, and thus the multiplicities of the eigenvalues of ζ_d if an s and/or a p electron is added to d^n.

If ζ_p is given a value of 2 and all the other parameters equal zero, then the eigenvalues of d^np, $d^{n-1}sp$ and $d^{n-2}s^2p$ are just 1 and -2 by (66). For a particular J, the multiplicity of the eigenvalue 1 equals the number of times the electron p is coupled with j equal 3/2 to the core d^n, $d^{n-1}s$, and $d^{n-2}s^2$, respectively. Similarly, the multiplicity of the eigenvalue -2 equals the number of times the electron p is coupled with j equal 1/2 to the core d^n, $d^{n-1}s$ and $d^{n-2}s^2$, respectively, for the particular J considered.

In our case we also combined the checks of ζ_d and ζ_p by letting ζ_d equal 20 and ζ_p equal 2.

The expected eigenvalues and their respective multiplicities are obtained by the same considerations as above.

Tables 7, 10, 13, 16, and 19 give the eigenvalues and their respective multiplicities for the configurations $(d+s)^np, 2 \leq n \leq 6$ when ζ_d equals 20.

Tables 8, 11, 14, 17, and 20 give the eigenvalues and their respective multiplicities for the configurations $(d+s)^np, 2 \leq n \leq 6$ when ζ_p equals 2.

Tables 6, 9, 12, 15, 18, and 21 give the eigenvalues and their respective multiplicities for the configurations $(d+s)^np, 1 \leq n \leq 6$, in the combined check with ζ_d equal to 20 and ζ_p equal to 2.

It should be noted that in tables 7, 10, 13, 16, and 19 the column "Eigenvalue" gives the eigenvalues of s^2p,sp and p when ζ_p has a value of 2. These values are necessary in order to obtain the multiplicities of the eigenvalues for the case of ζ_p equal to 2, and for the combined check ζ_d equal to 20 and ζ_p equal to 2.

For five electrons d the combination $(3/2)^5$ does not occur because for j equal to 3/2 there are only 4 values of m_j and by Pauli's principle it is forbidden for two electrons to have the same values of $(nljm_j)$.

For $(d+s)^6p$ only the pertinent values for the configuration d^5sp are required since d^6p and d^4s^2p are equivalent to d^4p here.

TABLE 6. *Eigenvalues and their multiplicities for the combined* ζ_d, ζ_p *Check of* (d+s)p

Conf.	Eigenvalue \ J	0	1	2	3	4
sp	1		1	1		
	-2	1	1			
dp	21		1	1	1	1
	18			1	1	
	-29	1	1	1	1	
	-32		1	1		

TABLE 7. *Eigenvalues and their multiplicities for the* ζ_d *Check of* $(d+s)^2p$

n	Eigenvalue ζ_{d^n}	J Combinations	J_{d^n}	$J_s 2 - n_p$	Eigen-value	J total					
						$\frac{1}{2}$	$\frac{3}{2}$	$\frac{5}{2}$	$\frac{7}{2}$	$\frac{9}{2}$	$\frac{11}{2}$
0	0			3/2	1		1				
	0			1/2	−2	1					
1	20	5/2	5/2	2	1						
				1	1	1	3	4	3	1	
				1	−2						
	−30	3/2	3/2	0	−2	3	4	3	1		
2	40	$(5/2)^2$	0 2 4			2	3	3	3	2	1
				$\frac{3}{2}$	1						
	−10	(5/2) (3/2)	1 2 3 4			3	5	6	5	3	1
				$\frac{1}{2}$	−2						
	−60	$(3/2)^2$	0 2			2	3	2	1		

TABLE 8. *Eigenvalues and their multiplicities for the* ζ_p *Check of* $(d+s)^2p$

Conf.	J / Eigenvalue	1/2	3/2	5/2	7/2	9/2	11/2
s^2p	1		1				
	−2	1					
dsp	1	3	4	4	3	1	
	−2	1	3	3	1		
d^2p	1	4	7	7	6	3	2
	−2	3	4	4	3	2	

TABLE 9. *Eigenvalues and their multiplicities for the combined* ζ_d, ζ_p *Check of* $(d+s)^2p$

Conf.	J / Eigenvalue	1/2	3/2	5/2	7/2	9/2	11/2
s^2p	1		1				
	−2	1					
dsp	21	1	2	2	2	1	
	18		1	2	1		
	−29	2	2	2	1		
	−32	1	2	1			
d^2p	41	1	2	2	2	1	1
	38	1	1	1	1	1	
	−9	2	3	4	3	2	1
	−12	1	2	2	2	1	
	−59	1	2	1	1		
	−62	1	1	1			

TABLE 10. *Eigenvalues and their multiplicities for the ζ_d Check of* $(d+s)^3p$

n	Eigenvalue $\zeta_{d}n$	J Combinations	$J_{d}n$	J_s3-n_p	Eigenvalue	J Total 0	1	2	3	4	5	6	7
1	20	5/2	5/2	3/2	1		1	2	2	1			
	−30	3/2	3/2	1/2	−2	1	2	2	1				
	40	$(5/2)^2$	0 2 4	2	1	2	5	6	6	5	3	1	
2	−10	(5/2)(3/2)	1 2 3 4	1	1	3	8	11	11	8	4	1	
	−60	$(3/2)^2$	0 2	1	−2	2	5	5	3	1			
	60	$(5/2)^3$	3/2 5/2 9/2	0	−2	1	3	4	4	3	2	1	
	10	$(5/2)^2 3/2$	1/2 $(3/2)_2$ $(5/2)_2$ $(7/2)_2$ 9/2 11/2	3/2	1	3	8	11	11	9	6	3	1
3	−40	$5/2(3/2)^2$	1/2 3/2 $(5/2)_2$ 7/2 9/2			2	6	8	8	6	3	1	
	−90	$(3/2)^3$	3/2	1/2	−2	1	2	2	1				

TABLE 11. *Eigenvalues and their multiplicities for the ζ_p Check of* $(d+s)^3p$

Conf.	Eigenvalue \ J	0	1	2	3	4	5	6	7
ds^2p	1	1	2	2	2	1			
	−2		1	2	1				
d^2sp	1	4	11	14	13	9	5	2	
	−2	3	7	8	7	5	2		
d^3p	1	5	12	15	16	12	8	4	1
	−2	2	7	10	8	6	3	1	

TABLE 12. *Eigenvalues and their multiplicities for the combined ζ_d, ζ_p Check of* $(d+s)^3p$

Conf.	Eigenvalue \ J	0	1	2	3	4	5	6	7
ds^2p	21		1	1	1	1			
	18			1	1				
	−29	1	1	1	1				
	−32		1	1					
d^2sp	41	1	3	4	4	3	2	1	
	38	1	2	2	2	2	1		
	−9	2	5	7	7	5	3	1	
	−12	1	3	4	4	3	1		
	−59	1	3	3	2	1			
	−62	1	2	2	1				
d^3p	61	1	2	2	3	2	1	1	
	58		1	2	1	1	1		
	11	2	5	7	7	6	4	2	1
	8	1	3	4	4	3	2	1	
	−39	1	4	5	5	4	2	1	
	−42	1	2	3	3	2	1		
	−89	1	1	1	1				
	−92		1	1					

TABLE 13. *Eigenvalues and their multiplicities for the* ζ_d *Check of* $(d+s)^4p$

n	Eigenvalue d^n	J Combinations	J_{d^n}							$J_{s^{4-n}p}$	Eigenvalue	J Total							
												1/2	3/2	5/2	7/2	9/2	11/2	13/2	15/2
2	40	$(5/2)^2$	0		2		4			3/2	1	2	3	3	3	2	1		
	−10	$(5/2)\ 3/2$		1	2	3	4			1/2	−2	3	5	6	5	3	1		
	−60	$(3/2)^2$	0		2							2	3	2	1				
3	60	$(5/2)^3$		3/2	5/2		9/2			2	1	4	7	8	7	5	3	1	
	10	$(5/2)^2\ 3/2$	1/2	$(3/2)_2$	$(5/2)_2$	$(7/2)_2$	(9/2)	11/2		1	1	11	19	22	20	15	9	4	1
	−40	$5/2\ (3/2)^2$	1/2	3/2	$(5/2)_2$	7/2	9/2			1	−2	8	14	16	14	9	4	1	
	−90	$(3/2)^3$		3/2						0	−2	3	4	3	1				
4	80	$(5/2)^4$	0		2		4					2	3	3	3	2	1		
	30	$(5/2)^3\ 3/2$	0	1_2	2_2	3_3	4_2	5	6	3/2	1	7	12	14	13	10	6	3	1
	−20	$(5/2)^2(3/2)^2$	0_2	1	2_4	3_2	4_3	5	6	1/2	−2	8	14	16	15	11	7	3	1
	−70	$5/2\ (3/2)^3$		1	2	3	4					3	5	6	5	3	1		
	−120	$(3/2)^4$	0									1	1						

TABLE 14. *Eigenvalues and their multiplicities for the* ζ_p *Check of* $(d+s)^4p$

Conf.	J / Eigenvalue	1/2	3/2	5/2	7/2	9/2	11/2	13/2	15/2
d^2s^2p	1	4	7	7	6	3	2		
	−2	3	4	4	3	2			
d^3sp	1	17	27	31	28	19	11	5	1
	−2	9	17	18	14	10	5	1	
d^4p	1	12	23	25	23	17	11	4	2
	−2	9	12	14	13	9	4	2	

TABLE 15. *Eigenvalues and their multiplicities for the combined ζ_d, ζ_p Check of* $(d+s)^4p$

Conf.	J / Eigenvalue	1/2	3/2	5/2	7/2	9/2	11/2	13/2	15/2
d^2s^2p	41	1	2	2	2	1	1		
	38	1	1	1	1	1			
	−9	2	3	4	3	2	1		
	−12	1	2	2	2	1			
	−59	1	2	1	1				
	−62	1	1	1					
d^3sp	61	3	4	5	5	3	2	1	
	58	1	3	3	2	2	1		
	11	7	12	14	13	10	6	3	1
	8	4	7	8	7	5	3	1	
	−39	5	9	10	9	6	3	1	
	−42	3	5	6	5	3	1		
	−89	2	2	2	1				
	−92	1	2	1					
d^4p	81	1	2	2	2	1	1		
	78	1	1	1	1	1			
	31	4	8	9	8	7	4	2	1
	28	3	4	5	5	3	2	1	
	−19	5	9	10	10	7	5	2	1
	−22	3	5	6	5	4	2	1	
	−69	2	3	4	3	2	1		
	−72	1	2	2	2	1			
	−119		1						
	−122	1							

TABLE 16. *Eigenvalues and their multiplicities for the ζ_d Check of* $(d+s)^5p$

n	Eigen-value $\zeta_d n$	J Combi-nations	$J_d n$							$J_s 5-n_p$	Eigen-value	J Total								
												0	1	2	3	4	5	6	7	8
3	60	$(5/2)^3$		3/2	5/2		9/2					1	3	4	4	3	2	1		
	10	$(5/2)^2\,3/2$	1/2	$(3/2)_2$	$(5/2)_2$	$(7/2)_2$	9/2	11/2		3/2	1	3	8	11	11	9	6	3		1
	−40	$5/2\,(3/2)^2$	1/2	3/2	$(5/2)_2$	7/2	9/2					2	6	8	8	6	3	1		
	−90	$(3/2)^3$		3/2						1/2	−2	1	2	2	1					
4	80	$(5/2)^4$	0		2		4			2	1	2	5	6	6	5	3	1		
	30	$(5/2)^3\,3/2$	0	1_2	2_2	3_3	4_2	5	6	1	1	7	19	26	27	23	16	9	4	1
	−20	$(5/2)^2(3/2)^2$	0_2	1	2_4	3_2	4_3	5	6	1	−2	8	22	30	31	26	18	10	4	1
	−70	$5/2\,(3/2)^3$		1	2	3	4			0	−2	3	8	11	11	8	4	1		
	−120	$(3/2)^4$	0									1	2	1						
5	100	$(5/2)^5$			5/2								1	2	2	1				
	50	$(5/2)^4\,3/2$	1/2	$(3/2)_2$	$(5/2)_2$	$(7/2)_2$	9/2	11/2		3/2	1	3	8	11	11	9	6	3	1	
	0	$(5/2)^3(3/2)^2$	$(1/2)_2$	$(3/2)_3$	$(5/2)_4$	$(7/2)_3$	$(9/2)_3$	11/2	13/2			5	14	19	20	17	12	7	3	1
	−50	$(5/2)^2(3/2)^3$	1/2	$(3/2)_2$	$(5/2)_2$	$(7/2)_2$	9/2	11/2		1/2	−2	3	8	11	11	9	6	3	1	
	−100	$5/2\,(3/2)^4$			5/2								1	2	2	1				

TABLE 17. *Eigenvalues and their multiplicities for the ζ_p Check of* $(d+s)^5p$

Conf.	Eigenvalue \ J	0	1	2	3	4	5	6	7	8
d^3s^2p	1	5	12	15	16	12	7	4	1	
	−2	2	7	10	8	6	4	1		
d^4sp	1	12	35	48	48	40	28	15	6	2
	−2	9	21	26	27	22	13	6	2	
d^5p	1	7	21	28	29	25	16	9	4	1
	−2	4	11	17	17	12	8	4	1	

TABLE 18. *Eigenvalues and their multiplicities for the combined ζ_d, ζ_p Check of* $(d+s)^5$ p

Conf.	Eigenvalue \ J	0	1	2	3	4	5	6	7	8
d^3s^2p	61	1	2	2	3	2	1	1		
	58		1	2	1	1	1			
	11	2	5	7	7	6	4	2	1	
	8	1	3	4	4	3	2	1		
	− 39	1	4	5	5	4	2	1		
	− 42	1	2	3	3	2	1			
	− 89	1	1	1	1					
	− 92		1	1						
d^4sp	81	1	3	4	4	3	2	1		
	78	1	2	2	2	2	1			
	31	4	12	17	17	15	11	6	3	1
	28	3	7	9	10	8	5	3	1	
	− 19	5	14	19	20	17	12	7	3	1
	− 22	3	8	11	11	9	6	3	1	
	− 69	2	5	7	7	5	3	1		
	− 72	1	3	4	4	3	1			
	− 119		1	1						
	− 122	1	1							
d^5p	101		1	1	1	1				
	98			1	1					
	51	2	5	7	7	6	4	2	1	
	48	1	3	4	4	3	2	1		
	1	3	9	12	13	11	8	5	2	1
	− 2	2	5	7	7	6	4	2	1	
	− 49	2	5	7	7	6	4	2	1	
	− 52	1	3	4	4	3	2	1		
	− 99		1	1	1	1				
	− 102			1	1					

TABLE 19. *Eigenvalues and their multiplicities for the* ζ_d *Check of* d^5sp

Eigenvalue ζ_{d^5}	J Combinations	J_{d^5}	J_{sp}	Eigenvalue	J Total 1/2	3/2	5/2	7/2	9/2	11/2	13/2	15/2	17/2
100	$(5/2)^5$	5/2			1	3	4	3	1				
			2	1									
50	$(5/2)^4\,3/2$	1/2 $(3/2)_2$ $(5/2)_2$ $(7/2)_2$ 9/2 11/2			11	19	22	20	15	9	4	1	
			1	1									
0	$(5/2)^3(3/2)^2$	$(1/2)_2$ $(3/2)_3$ $(5/2)_4$ $(7/2)_3$ $(9/2)_3$ 11/2 13/2			19	33	39	37	29	19	10	4	1
			1	−2									
−50	$(5/2)^2(3/2)^3$	1/2 $(3/2)_2$ $(5/2)_2$ $(7/2)_2$ 9/2 11/2			11	19	22	20	15	9	4	1	
			0	−2									
−100	$5/2\,(3/2)^4$	5/2			1	3	4	3	1				

TABLE 20. *Eigenvalues and their multiplicities for the* ζ_p *Check of* d^5sp

Eigenvalue \ J	1/2	3/2	5/2	7/2	9/2	11/2	13/2	15/2	17/2
1	15	28	34	29	20	12	5	1	
−2	28	49	57	54	41	25	13	5	1

TABLE 21. *Eigenvalues and their multiplicities for the combined* ζ_d, ζ_p *Check of* d^5sp

Eigenvalue \ J	1/2	3/2	5/2	7/2	9/2	11/2	13/2	15/2	17/2
101	1	2	2	2	1				
98		1	2	1					
51	7	12	14	13	10	6	3	1	
48	4	7	8	7	5	3	1		
1	12	21	25	24	19	13	7	3	1
−2	7	12	14	13	10	6	3	1	
−49	7	12	14	13	10	6	3	1	
−52	4	7	8	7	5	3	1		
−99	1	2	2	2	1				
−102		1	2	1					

7. Checks for the Relative Phases of the Electrostatic and Spin-Orbit Interactions

Since the matrices of the electrostatic interaction and the spin-orbit interaction do not generally commute, it is difficult to find values of the parameters which yield simple eigenvalues. The matrices which do commute are the electrostatic matrices of $(d+s)^n$ and the matrices of ζ_p.

Now, if we check the relative phases of the electrostatic matrices of $(d+s)^n$ and the matrices of ζ_p, we also know that the relative phases of the electrostatic matrices of $(d+s)^n$ and ζ_d are correct. This follows from the previous check where the relative phases of the matrices of ζ_d and ζ_p are checked. The relative phases of the matrices of the interactions $d-p$ and/or $s-p$ and the electrostatic matrices of $(d+s)^n$ are checked in the Casimir [1], and the ^{1}P Checks. Thus, if in addition to the other checks, the Check $(d+s)^n+\zeta_p$ is considered, then we have a verification of the correctness of the relative phases of all the electrostatic and spin-orbit interaction matrices.

For $(d+s)^n$ the parameters of the Casimir Check, as obtained from (30) [1], are used:

$$
\begin{aligned}
A &= 11n \\
S' &= 9 \\
S'' &= 34-8n \\
B &= B' = B'' = 1 \\
G'_{ds} &= 8 \\
\alpha &= \frac{3}{2} \\
H &= H' = \frac{2\sqrt{10}}{5}
\end{aligned}
\tag{67}
$$

We note that it is necessary to replace λ by α, since $L(L+1)$ refers to the configuration $(d+s)^n$ here.

To ζ_p a value of 2 is given as before.

The expected eigenvalues for each term of $(d+s)^n$ are given in [1], (pp. 33-35). Then to find the eigenvalues of $(d+s)^n p$ we simply add to the eigenvalues of $(d+s)^n$ a value of 1 or -2 depending upon whether the electron p is coupled as j equal to 3/2 or j equal to 1/2 respectively, for a particular level of $(d+s)^n p$.

As an example consider the expected eigenvalues of $(d+s)^2 p$ for J equal to 1/2. From [1] the expected eigenvalues can only have the values 57, 54, 33, 30, 21, and 18. The eigenvalue 57 can only be obtained from

$$(d+s)^2\ {}^1\mathrm{D}_2 + p_{3/2}.$$

The eigenvalue 54 can be obtained from

$$(d+s)^2\ {}^1\mathrm{S}_0 + p_{1/2}.$$

The eigenvalue 33 has a multiplicity of 5:

$$(d+s)^2\ {}^3\mathrm{P}_{1,2} + p_{3/2},\ (d+s)^2\ {}^3\mathrm{D}_{1,2} + p_{3/2},\ (d+s)^2\ {}^3\mathrm{F}_2 + p_{3/2}.$$

The eigenvalue 30 has a multiplicity of 3:

$$(d+s)^2\ {}^3\mathrm{P}_{0,1} + p_{1/2},\ (d+s)^2\ {}^3\mathrm{D}_1 + p_{1/2}.$$

The eigenvalue 21 can only be obtained from

$$(d+s)^2\ {}^1\mathrm{D} + p_{3/2}.$$

The eigenvalue 18 can be obtained from

$$(d+s)^2\ {}^1\mathrm{S} + p_{1/2}.$$

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8. References

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