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Original Contribution

APPLICATION OF MATHEMATICS CALCULATION FOR MICROSTATES AND DESCRIPTION OF THE p^2 ELECTRON CONFIGURATION

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ABSTRACT

The aim of this research was to compute the number of microstates for p^2 configuration $n=6$ and $x=2$, for d^2 configuration $n=10$ and $x=2$ and f^2 configuration $n=14$ and $x=2$ using Euclidean vectors and the math function factorial as well as to describe in detail the microstates for p^2 configuration $n=6$ and $x=2$. The following results were obtained: for p^2 configuration $n=6$ and $x=2$, $N=15$ microstates; for d^2 configuration $n=10$ and $x=2$, $N=45$ microstates; for f^2 configuration $n=14$ and $x=2$, $N=91$ microstates. It was established that the 15 microstates of the p^2 configuration. It was found that the 15 microstates of the p^2 electron configuration belonged to three terms as followed: 5 microstates corresponding to the ^1D term; 9 microstates to the ^3P term and 1 microstate to the ^1S term.

Key words: vector, factorial, microstate, p^2 electron configuration

INTRODUCTION

Linear algebra and analytical geometry theory and methods are increasingly applied in chemistry. The states of multi-electron atoms or ions in chemistry are described and classified by two schemes (Russell-Saunders (L-S) and j-j coupling schemes). Both use vectors and factorials.

1. Vectors

Definitions

- A *vector* is a geometric object that has both magnitude (length) and direction.
- The *tail* of the vector is the end opposite the arrow. It represents where the vector is moving from.
- The *head* of the vector is the end with the arrow. It represents where the vector is moving to.
- The *zero vector* is denoted $\vec{o}$. It has zero length and all the properties of zero.
- Two vectors are *equal* is they have both the same magnitude and the same direction.
- Two vectors are *parallel* if they have the same $(\uparrow\uparrow$ or $\downarrow\downarrow)$ or opposite $(\uparrow\downarrow)$ directions. That is, if the angles of the vectors are the same or 180^0 different.
- Two vectors are *perpendicular* if the difference of the angles of the vectors is 90^0 or 270^0 (1-4).

Magnitude of a Vector

The magnitude of a vector $\overrightarrow{AB}$ is the distance between the initial point $A(x_1, y_1)$ and the end point $B(x_2, y_2)$. In symbols the magnitude of $\overrightarrow{AB}$ is written as $\left|\overrightarrow{AB}\right|$. If the coordinates of the initial point and the end point of a vector are given, the *distance formula* can be used to find its magnitude: $\left|\vec{\mathbf{v}}\right| = \left|\overrightarrow{AB}\right| = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$

(Figure 1).

Let as remark, that $\left|\overrightarrow{AB}\right| = \left|\overrightarrow{BA}\right|$. The directions of the two vectors are opposite, but their magnitudes are the same (1-4).

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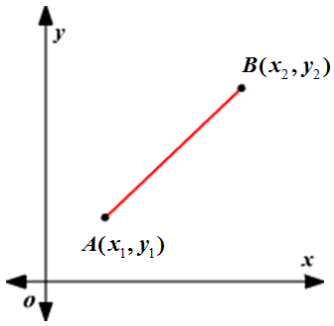


Figure 1. Magnitude of a vector.

Direction of a Vector

The direction of a vector is the measure of the angle it makes with a *horizontal line*. One of the following formulas can be used to find the direction of a vector:

$$\tan\theta = \frac{y}{x},$$

where x is the horizontal change and y is the vertical change or

$$\tan\theta = \frac{y_2 - y_1}{x_2 - x_1},$$

where (x_1, y_1) is the initial point and (x_2, y_2) is the terminal point (1-4).

Operations with Vectors

It is possible to operate with vectors in some of the same ways we operate with numbers. In particular:

Adding and Subtracting Vectors

To add or subtract two vectors, add or subtract the corresponding components.

Let $\vec{\mathbf{u}} = \langle u_1, u_2 \rangle$ and $\vec{\mathbf{v}} = \langle v_1, v_2 \rangle$ be two vectors. Then, the sum of $\vec{\mathbf{u}}$ and $\vec{\mathbf{v}}$ is the vector

$$\vec{\mathbf{u}} + \vec{\mathbf{v}} = \langle u_1, u_2 \rangle + \langle v_1, v_2 \rangle = \langle u_1 + v_1, u_2 + v_2 \rangle.$$

The difference of $\vec{\mathbf{u}}$ and $\vec{\mathbf{v}}$ is

$$\vec{\mathbf{u}} - \vec{\mathbf{v}} = \vec{\mathbf{u}} + (-\vec{\mathbf{v}}) = \langle u_1 - v_1, u_2 - v_2 \rangle.$$

The sum of two or more vectors is called the resultant. The resultant of two vectors can be found using either the *parallelogram method* or the *triangle method*.

Parallelogram Method:

Draw the vectors so that their initial points coincide. Then draw lines to form a complete parallelogram. The diagonal from the initial point to the opposite vertex of the parallelogram is the resultant.

Vector Addition:

1. Place both vectors $\vec{\mathbf{u}}$ and $\vec{\mathbf{v}}$ at the same initial point.
2. Complete the parallelogram. The resultant vector $\vec{\mathbf{u}} + \vec{\mathbf{v}}$ is the diagonal of the parallelogram **(Figure 2).**

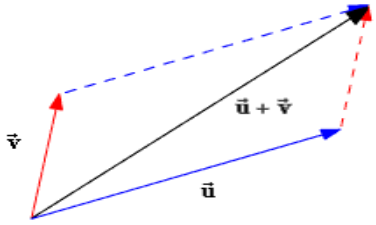


Figure 2. Vector Addition

Vector Subtraction:

3. Complete the parallelogram.
4. Draw the diagonals of the parallelogram from the initial point **(Figure 3)**.

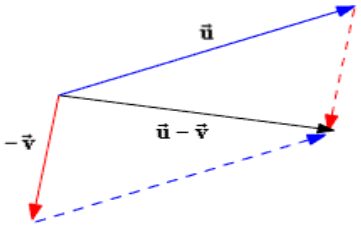


Figure 3. Vector Subtraction

Triangle Method:

Draw the vectors one after another, placing the initial point of each successive vector at the terminal point of the previous vector. Then draw the resultant from the initial point of the first vector to the terminal point of the last vector. This method is also called the *head-to-tail method* **(Figures 4, 5).**

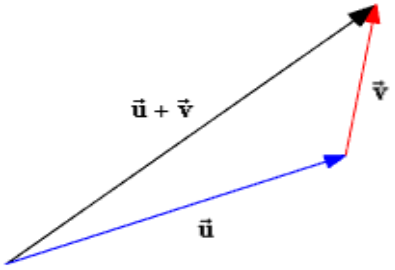


Figure 4. Vector Addition.

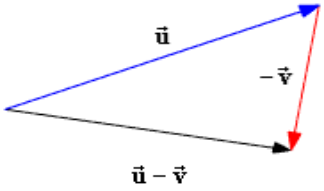


Figure 5. Vector Subtraction.

Vector Algebra

$\vec{u}+\vec{v}=\vec{v}+\vec{u}$	$\vec{u}+(-\vec{u})=\vec{o}$	$a.(\vec{u}+\vec{v})=(a.\vec{u})+(a.\vec{v})$
$(\vec{u}+\vec{v})+\vec{w}=\vec{u}+(\vec{w}+\vec{v})$	$0.\vec{u}=\vec{o}$	$(a+b).\vec{u}=(a.\vec{u})+(b.\vec{u})$
$\vec{u}+\vec{o}=\vec{u}$	$1.\vec{u}=\vec{u}$	$(ab).\vec{u}=a.(b.\vec{u})=b.(a.\vec{u})$

Scalar Multiplication

Scalar multiplication changes the magnitude of a vector, but not the direction. In general,

$\vec{u}=\langle u_1,u_2\rangle$ $\qquad k.\vec{u}=\langle k.u_1,k.u_2\rangle$

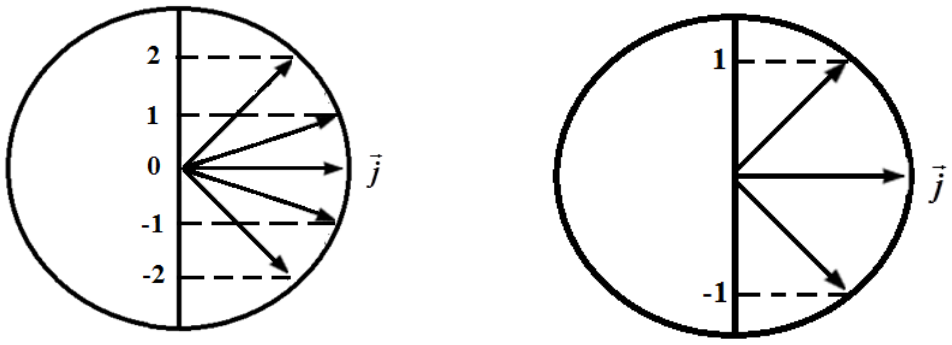
2. Factorial

In mathematics, the *factorial* of a non-negative integer n, denoted by $n!$, is the product of all positive integers less than or equal to n, e.t. $n!=1.2\ldots(n-2).(n-1).n$. In a particular way $0!=1!=1$ (1-4).

The aim of this research was to calculate the number of microstates for p^2 configuration $n=6$ and $x=2$, for d^2 configuration $n=10$ and $x=2$ and f^2 configuration $n=14$ and $x=2$ using Euclidean vectors and the math function factorial as well as to describe in detail the microstates for p^2 configuration $n=6$ and $x=2$.

MATERIAL AND METHODS

It is acknowledged that the movement of an electron in an atom could be represented by the orbital angular momentum. Similarly, the intrinsic motion of the electron is given by the spin angular momentum**.** Both angular momenta should be presented by vectors which have length and direction. Vectors will be identified by letters, their projections with m (for a single electron) or M (for more than 1 electron), and lengths will be represented by $|m|$ and $|M|$, respectively. For an electron with quantum numbers *l* and *s*, and orbital and spin angular momenta $\vec{l}$ and $\vec{s}$, the total angular momentum describing both motions is a sum of vectors: $\vec{j}=\vec{l}+\vec{s}$ (5-10). Both vectors process (rotation of an vector around an axis with only vectors' initial point lying on the axis; the vector and the axis are under a specific angle). Due to this motion, both vectors described a cone each. The addition of $\vec{l}$ and $\vec{s}$ could not be random. The angle between them remains constant in the course of processing. This results from the strict spatial orientation of both vectors. They could be oriented in a way such as their vector sum has strictly defined values of $\vec{j}$ projections. Also, the differences between these projections *(h)* should be integers (11-19). The above mentioned is illustrated on **Figure 6** for an electron on p-AO.



$|\vec{l}|=1,\ |\vec{s}|=\frac{1}{2},\ |\vec{j}|=\frac{3}{2}$ $\qquad$ $|\vec{l}|=1,\ |\vec{s}|=-\frac{1}{2},\ |\vec{j}|=\frac{1}{2}$.

Figure 6. Addition of vectors of orbital and spin angular momenta for $|\vec{l}|=1$ and $|\vec{s}|=1/2$. Both circles represent the space quantization of the total angular momentum $\vec{j}$. The lengths of vectors are shown below the circles.

Figure 7 depicts the addition of $\vec{L}$ and $\vec{S}$ for 2 electrons on p-AO.

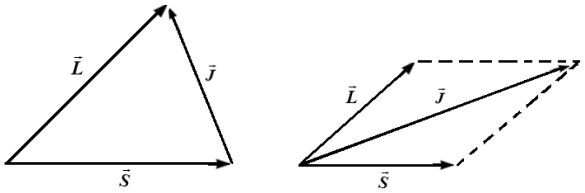


Figure 7. Addition of vectors of orbital angular momentum $\vec{l}$ and spin angular momentum $\vec{s}$ for $\left|\vec{l}\right|=1$ and $\left|\vec{s}\right|=1$.

The total angular momentum $\vec{j}$ or $\vec{J}$ for one or more electrons, respectively is quantized in space in the same way, as shown on both figures.

Russell-Saunders coupling scheme. LS scheme

In the Russell-Saunders scheme, the spin and orbital angular momenta are always summed independently: $\vec{L}=\vec{l}_1+\vec{l}_2+\ldots+\vec{l}_N=\sum_{i=1}^{N}\vec{l}_i$,

$\vec{S}=\vec{s}_1+\vec{s}_2+\ldots+\vec{s}_N=\sum_{i=1}^{N}\vec{s}_i$.

Then the resulting two vectors $\vec{L}$ and $\vec{S}$ are combined to obtain the total angular momentum $\vec{J}$: $\vec{J}=\vec{L}+\vec{S}$.

j-j coupling scheme

The combination of angular momenta of a multi-electron atom according to the j-j coupling scheme is done by combining each individual orbital to respective spin momentum $\vec{j}_i=\vec{l}_i+\vec{s}_i$ and thereafter, the total angular momentum is obtained as the sum of individual total angular momenta: $\vec{J}=\vec{j}_1+\vec{j}_2+\ldots+\vec{j}_N=\sum_{i=1}^{N}\vec{j}_i$

This order of combining is derived from the nature of the j-j scheme – each electron determines its own momentum, and then follow the combination of total individual angular momenta of all electrons.

The spin multiplicity is denoted with 2S + 1. It is added as a superscript to the left of the letter expressing the sum of orbital momenta (electron state). For example, the electron state derived from the electronic configuration $1s^1$ is:

$s=1/2 \qquad l=0 \qquad 2s+1=2 \qquad {}^2S$.

The symbol ^{2}S (read as doublet es) is an electron term derived from the electronic configuration $1\ s^1$ and including two microstates:

$m_s=1/2 \qquad m_l=0;$

$m_s=-1/2 \qquad m_l=0.$

The six microstates of the electronic configuration $2p^1$ are:

$m_s=+1/2 \qquad m_l=1,0,-1;$

$m_s=-1/2 \qquad m_l=1,0,-1.$

They could be grouped into:

$s=1/2 \qquad l=1 \qquad 2s+1=2 \qquad \text{term.}\ {}^2P$.

The symbol ^{2}P (read as doublet pe), and ^{2}S (read as doublet es) are called electron terms. Therefore, electron terms are a group of microstates (or combinations between them) with the same energy.

The Russell Saunders scheme could be illustrated with several examples:

Closed shell — the general rule for this shell type that it always has S = 0 and L = 0 or term ^{1}S.

Open shell — only one of atomic orbitals making up a given electronic configuration without the maximum number of electrons is enough to have an open shell..

The total number of microstates for any configuration can be counted using by following expression (20).

Number of ways of filling electrons N:

$$N=\frac{2(2l+1)!}{x!\left(2(2l+1)!-x!\right)} \text{ or } \frac{n!}{x!(n!-x!)}$$

n = 2(2*l*+1) or double of the total number of orbital's (For s-AO = 2, p-AO = 6, d-AO = 10, f-AO = 14)

x = Total number of electrons in sub shell.

RESULTS AND DISCUSSION

So, for p^2 configuration $n=6$ and $x=2$

$$N=\frac{6!}{2!(6!-2!)},\ N=\frac{6.5.4.3.2.1}{4.3.2.1.2.1},$$

$N=15$ Microstates.

For d^2 configuration $n=10$ and $x=2$

$$N=\frac{10!}{2!(10!-2!)},\ N=\frac{10.9.8.7.6.5.4.3.2.1}{8.7.6.5.4.3.2.1.2.1},$$

$N=45$ Microstates.

For f^2 configuration $n=14$ and $x=2$

$$N=\frac{14!}{2!(14!-2!)},$$

$$N=\frac{14.13.12.11.10.9.8.7.6.5.4.3.2.1}{12.11.10.9.8.7.6.5.4.3.2.1.2.1},$$

$N=91$ Microstates.

On **Figure 8** and **Table 1** we present 15 microstates obtained for p^2 configuration $n=6$ and $x=2$.

In **Table 1** M_L and M_S denote the projections of respective $\vec{L}$ and $\vec{S}$ vectors. The content of the table becomes clear from Fig. 8 – the numbers 1, 0, -1 are the m_l-projections of the orbital angular momenta of the first and second electron, the signs (+) and (-), placed over m_l indicate the m_s-projections of the spin angular momentum.

Table 1. Microstates of the electronic configuration p^2

	M_S		
M_L	1	0	-1
2		$\left(\overset{+}{1},\overset{-}{1}\right)$	
1	$\left(\overset{+}{1},\overset{+}{0}\right)$	$\left(\overset{+}{1},\overset{-}{0}\right),\left(\overset{-}{1},\overset{+}{0}\right)$	$\left(\overset{-}{1},\overset{-}{0}\right)$
0	$\left(\overset{+}{1},\overset{+}{-1}\right)$	$\left(\overset{+}{1},\overset{-}{-1}\right),\left(\overset{+}{0},\overset{-}{0}\right),\left(\overset{-}{1},\overset{+}{-1}\right)$	$\left(\overset{-}{1},\overset{-}{-1}\right)$
-1	$\left(\overset{+}{0},\overset{+}{-1}\right)$	$\left(\overset{+}{0},\overset{-}{-1}\right),\left(\overset{-}{0},\overset{+}{-1}\right)$	$\left(\overset{-}{0},\overset{-}{-1}\right)$
-2		$\left(\overset{+}{-1},\overset{-}{-1}\right)$	

For instance, for $m_{l_1}=1,\ m_{l_2}=0,\ m_{s_1}=1/2$ and $m_{s_2}=1/2$, the microstate is $\left(\overset{+}{1},\overset{+}{0}\right)$,

whose wave function is $\psi_1=\phi_{m_l}s_1\phi_{m_l}s_2=\overset{+}{\phi}\overset{+}{\phi}_0$

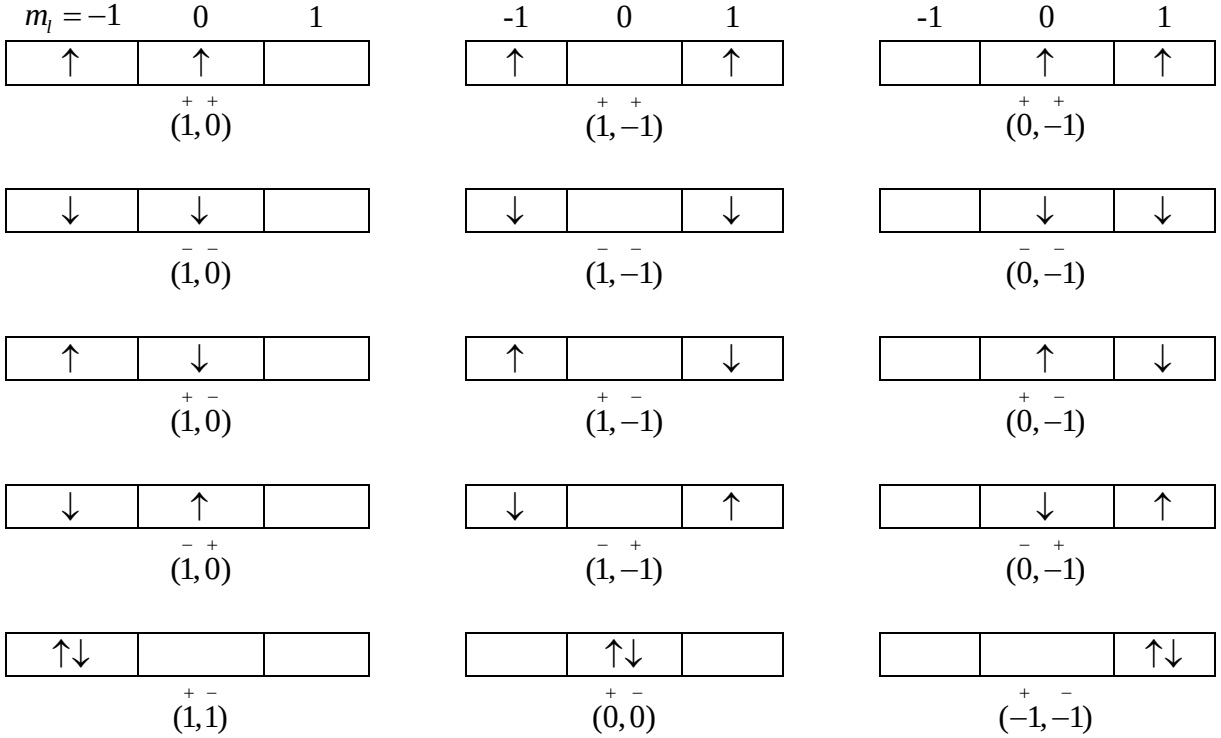


Figure 8. Microstates which are derived from the electronic configuration p^2.

A more complex problem arises for wave functions of the second column, where there are two or three microstates within a cell.
Let's take a look on the content of the cell with $M_L = 1$ $M_s = 0$.

There are two microstates - $\left(\overset{+}{1},\overset{-}{0}\right)$ and $\left(\overset{-}{1},\overset{+}{0}\right)$.

They could be written as functions

$$\psi_1 = c_1\left(\overset{+}{1},\overset{-}{0}\right) + c_2\left(\overset{-}{1},\overset{+}{0}\right),$$

$$\psi_2 = c_3\left(\overset{+}{1},\overset{-}{0}\right) + c_4\left(\overset{-}{1},\overset{+}{0}\right),$$

the coefficients $c_1, c_2, c_3,$ and c_4 are associated with the conditions

$c_1^2 + c_2^2 = 1$ $\quad$ $c_3^2 + c_4^2 = 1$ norming

$c_1^2 + c_3^2 = 1$ $\quad$ $c_2^2 + c_4^2 = 1$ distribution,

reflecting the circumstance that both functions are normed and that every microstate is distributed between both functions in a way such that it is completely depleted.
The system of 4 equations shown above with four variables has a solution

$c_1^2 = c_4^2$ and $c_2^2 = c_3^2$, hence $|c_1| = |c_4|$ и $|c_2| = |c_3|$,

but it is impossible to find the numeric values – the four equations are not linearly independent.

So, we will proceed as follows.
By definition, the electron term comprises the microstates or microstate combinations having the same energy. It follows that one of the ψ_1 or ψ_2 functions with the respective values of coefficients must yield the same energy as $\left(\overset{+}{1},\overset{+}{0}\right)$ and $\left(\overset{-}{1},\overset{-}{0}\right)$, which are within the same row in the first and third column. The other combination should have an energy different from the first one, corresponding to another electron term. It could be easily deduced that this is the energy of the microstates $\left(\overset{+}{1},\overset{-}{1}\right)$ and $\left(\overset{+}{-1},\overset{-}{-1}\right)$ from the first and last row of the same (middle) column.

Let's now take a look on **Table 1** from another aspect. If we begin with the microstate with highest M_L value – this is $\left(\overset{+}{1},\overset{-}{1}\right)$, after addition of the two vectors, each with length $\sqrt{2}$ and projection on the selected axis 1, we obtain a vector with length of $\sqrt{6}$ and projection on the same axis 2 (in $h/2\pi$ units).

In other words, the microstate $\left(\overset{+}{1},\overset{-}{1}\right)$ has to be a function of this vector. Once obtained however, this vector is quantized in the space and apart the projection +2, it could be also oriented in a way such as to have projections equal to +1, 0, -1, -2. Also, the orientation of the spins of both electrons should be always opposite. It is important to understand that one of respective combinations in the column with Ms = 0 belongs to the vector derived from $\left(\overset{+}{1},\overset{-}{1}\right)$. This vector is denoted with the letter D.

The spin multiplicity is 2S+1=1, or there is one term ^{1}D (singlet de), which includes 5 microstates or combinations, all of which (without exceptions) are arranged vertically in the middle column of **Table 1.**

As these combinations are unknown to us, we will randomly remove one microstate from each row of the second column as belonging to the term ^{1}D. The result is illustrated in the new **Table 2.**

With the new table, we proceed in the same way as with **Table 1** – choosing the microstate with highest value for M_L. These are $\left(\overset{+}{1},\overset{+}{0}\right)$, $\left(\overset{+}{1},\overset{-}{0}\right)$, $\left(\overset{-}{1},\overset{-}{0}\right)$. From them, we retain the microstate with maximum value for M_S, i.e. $\left(\overset{+}{1},\overset{+}{0}\right)$. It corresponds to M_L = 1 and M_S = 1 or it is derived from vectors $\vec{L}$ and $\vec{S}$ each with a length of $\sqrt{2}$, whose projections could be 1, 0, -1. These two vectors determine the existence of nine microstates with different energy, differing in projections on a random axis. These nine microstates constitute the electron term ^{3}P. If these microstates (or their combination in the middle column) are removed from **Table 2**, only one combination of microstates is left, which is not mentioned so far and whose energy in different from the energy of ^{1}D and ^{3}P terms. It is

$$3^{-1/2}\left[\left(\overset{+}{0},\overset{-}{0}\right) - \left(\overset{+}{1},\overset{-}{-1}\right) - \left(\overset{+}{-1},\overset{-}{1}\right)\right]$$

and due to the fact that it has M_L = 0 and M_S = 0, it forms the term ^{1}S.

Table 2. *Microstates of p^2 after removing ^1D.*

	M_s		
M_L	1	0	-1
2			
1	$\binom{+\ +}{1,0}$	$\binom{+\ -}{1,0}$	$\binom{-\ -}{1,0}$
0	$\binom{+\ +}{1,-1}$	$\binom{+\ -}{0,0}, \binom{-\ +}{1,-1}$	$\binom{-\ -}{1,-1}$
-1	$\binom{+\ +}{0,-1}$	$\binom{-\ +}{0,-1}$	$\binom{-\ -}{0,-1}$
-2			

CONCLUSIONS

Ultimately, the description of the 15 microstates derived from the electronic configuration P^2 led to the following result. These microstates fell into three energy terms as follows:

- 5 microstates included in the electron term ^1D;
- 9 microstates included in the electron term ^3P;
- 1 microstates included in the electron term ^1S.

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