

 <p>ISSN NO. 2320-5407</p>	<p>Journal Homepage: - www.journalijar.com</p> <h2 style="text-align: center;">INTERNATIONAL JOURNAL OF ADVANCED RESEARCH (IJAR)</h2> <p style="text-align: center;">Article DOI: 10.21474/IJAR01/8810 DOI URL: http://dx.doi.org/10.21474/IJAR01/8810</p>	
---	--	---

RESEARCH ARTICLE

WAVEFUNCTIONS FOR CONFIGURATION $4f^2 5d 6s^2$ OF PRASEODYMIUM (Pr I) TO CALCULATE ENERGY AND OTHER SPECTROSCOPIC QUANTITIES.

Roohi Zafar^{1,2}, Saba Javaid^{1,2} and Zaheer uddin².

1. NED University of Engineering and Technology.
2. Department of Physics, University of Karachi.

Manuscript Info

Manuscript History

Received: 04 February 2019

Final Accepted: 06 March 2019

Published: April 2019

Key words:-

LS terms, coefficient of fractional parentage, equivalent and non-equivalent electrons, coupled wavefunction.

Abstract

Term symbols are used to label characteristics of atomic and ionic levels. The information we extract from term symbols are spin multiplicity, orbital and total angular momentum for different electronic states of atoms as well as its ions. wave function can be written as a linear combination of the pure parentage wave functions for the specific terms having same total orbital angular momentum L and total spin angular momentum S. These wavefunctions are important to calculate because several spectroscopic quantities e.g. energy, transition probability etc. can be calculated with the help of these wavefunctions. In this study the 42 electronic terms of configurations, 102 the possible electronic state and 23 coupled wavefunctions of the terms of $4f^2 5d 6s^2$ configuration of Pr I, with seven parents (1S , 1D , 1G , 1I , 3P , 3F , 3H) belonging to f^2 are reported.

Copy Right, IJAR, 2019,. All rights reserved.

Introduction:-

Praseodymium belongs to the Lanthanide group. Lanthanides in their ground state electronic configuration have a closed 6s electron shell but an open 4f shell. They are very important to study because of their use in daily life. As a metal, praseodymium is used in making alloys and optical glasses. Pr is abundant in the Sun and in some peculiar stars therefore the spectrum of praseodymium is also of interest to Astrophysicists. Due to its open 4f shell Praseodymium atom (Pr I) has a large number of fine structure (fs) levels among which approximately more than 3000 levels are known which but still a huge number of them are unknown.

The spectrum of praseodymium (Pr I and Pr II) have been widely studied by a number of authors by using wide range of experimental techniques. Several studies on the electronic configuration of Pr were collected and published in 1978 (W. C. Martin et al., 1978). An important contribution to the investigation of the spectrum of praseodymium came from the work of A. G. G. G. (Ginibre, A., 1981, Ginibre, A., 1989). She used a high-resolution Fourier transform (FT) spectrum of praseodymium to discover new levels of Pr I and Pr II. In 2006 Furmann et al (Furmann et al., 2006) also discovered a large number of new fine structure levels of praseodymium having both even and odd parity configuration. With the help of these discovered levels, they classified a large number of spectral lines in the spectrum of Pr I. In 2011 a new highly resolved Fourier transformed spectra of Pr atom were recorded by A. Gamper et al. and with the help of this spectra they found around 9000 new lines of Pr and classified 1194 lines as transitions between energy levels of the Pr atom and 19 as transitions of the Pr ion (Gamper et al., 2011). In 2012, 2014 and 2015 by using laser induced fluorescence (LIF) spectroscopy technique Zaheer et al reported new levels of Pr (Uddin et al., 2012, 2014, 2015). In 2014, 66 even and 58 odd parity fine structure levels of Pr I were discovered

Corresponding Author:- Roohi Zafar.

Address:- NED University of Engineering and Technology.

by Siddiqui, Shamim and Windholz (Siddiqui, I. et al., 2014). In 2016 Siddiqui et al. discovered new fine structure energy levels of Pr I of medium angular momentum quantum number (Siddiqui et al., 2016). In 2016 Shamim et al. also published 32 new even parity level and 38 odd parity level and in the same Siddiqui, I. et al. also discovered new levels of Pr I with medium angular momentum quantum number year (Khan et al. 2016). In 2017 L.M. Sobolewski et al. investigated 52 lines of Pr I using LIF method, they also reported Landé g factor of 71 levels of Pr I (Sobolewski et al., 2017)

In this work, by using Russell-Saunders LS coupling scheme term values of configuration $4f^25d6s^2$ of Pr I with their angular momentum were and coefficient of Fractional parentage is calculated and with the help of these coefficient ortho-normalized states of $4f^25d6s^2$ configuration is generated.

Methodology:-

The Russell Saunders coupling method was used first to calculate terms arising from equivalent electron by taking Pauli's Principle into account; the results are then combined with other non-equivalents electrons (Murthy et al. 2017, Meena et al. 2013, Bransden, 2003). For configuration $4f^25d6s^2$, the coupling is done in three steps; first the terms of f^2 and s^2 were found then result of f^2 were combined with the terms of d and finally f^2d terms were combined with term of s^2 . To calculate the coupled wavefunction of configuration $4f^25d6s^2$ of Pr I, coefficient of fractional parentage method is applied. In this technique one selects a trial principle parents given to calculate whether a given principle produces non-zero and independent coefficient of fractional parentage. These wavefunctions are given as follows;

$$|a^n b^n; (S_o L_o) \alpha SL \rangle = \sum_{\alpha' L' S'} (a^n b^n \alpha SL \{ a^n \alpha' L' S', b^n \} | a^n b^n; (L' S') SL \rangle \quad (i)$$

here $(a^n b^n \alpha SL \{ a^n \alpha' L' S', b^n \})$ is the coefficient of fractional parentage. The wavefunction arises from configuration $a^n b^n$ is written as $|a^n b^n; (S_o L_o) \alpha SL \rangle$, here symbol S_o, L_o are used for principal parents spin and orbital angular momenta, S and L are the spin and orbital angular momenta of the resultant term of the configuration and $L' S'$ are used for parents over which summation is applied. The final term wavefunction is a linear combination of wavefunctions $|a^n b^n; (L' S') SL \rangle$. In order to find the coefficient of wavefunctions $|a^n b^n; (L' S') SL \rangle$ a method given in (Condon et al., 1980, Cowan et al., 1981, Racah G. 1943) is applied. The calculated wavefunctions are normalized.

Result and Discussion:-

There are 42 terms value and 102 number of levels generated in this configuration. The terms arising from $4f^25d6s^2$ configurations are given in tables I and the number of electronic states is given in table II, respectively. In $4f^25d6s^2$ configuration, the S orbital is completely filled, it does not contribute in final terms. Therefore f^2d orbitals are used to calculate the coefficient of fractional parentage of final term. To generate the wavefunctions, f^2 was used as parent configuration, which generated seven terms of parent ($^1S, ^1D, ^1G, ^1I, ^3P, ^3F, ^3H$). The choice of seven term as principle parents gives the coefficient of fractional parentage for 23 LS state of $4f^25d6s^2$ configuration. Repeated final terms wavefunctions are non-orthogonal, they may be orthogonalized by using Gram Schmidt procedure. The choice of some terms as principle parents has zero coefficient of fractional. The coefficient of fractional parentage of term $^2D, ^2F$ and 2G are given in table III, IV and V respectively. Table III shows that only $^1D, ^3P$ contributing as a principle parents in constructing 2D wavefunction. Similarly, in table IV zero contribution of $^1S, ^1I, ^3H$ as a principle parent in 2F coupled wavefunction. Twenty-three calculated wavefunction are normalized and are given in table VI.

Table I: Terms value with their quantity of configuration $4f^25d6s^2$

Term	2S	2P	2D	2F	2G	2H	2I	2K	2L
quantity	1	3	5	5	5	4	3	2	1
Term	4S	4P	4D	4F	4G	4H	4I	4K	
quantity	0	2	2	3	2	2	1	1	

Table II: Angular momentum with allowed terms value with their parents for configuration $4f^25d6s^2$

J	Frequency	Allowed Terms						
0.5	8	$(^1D)^2S$	$(^1D)^2P$	$(^3P)^2P$	$(^3F)^2P$	$(^3P)^4P$	$(^3F)^4P$	$(^3P)^4D$
		$(^3F)^4D$						

1.5	15	$(^1D)^2P$	$(^3P)^2P$	$(^3F)^2P$	$(^1S)^2D$	$(^1D)^2D$	$(^1G)^2D$	$(^3P)^2D$
		$(^3P)^4P$	$(^3F)^4P$	$(^3P)^4D$	$(^3F)^4D$	$(^3P)^4F$	$(^3F)^4F$	$(^3H)^4F$
		$(^3F)^2D$						
2.5	17	$(^1S)^2D$	$(^1D)^2D$	$(^1G)^2D$	$(^3P)^2D$	$(^3F)^2D$	$(^1D)^2F$	$(^1G)^2F$
		$(^3F)^2F$	$(^3H)^2F$	$(^3P)^4P$	$(^3F)^4P$	$(^3P)^4D$	$(^3F)^4D$	$(^3P)^4F$
		$(^3H)^4F$	$(^3P)^2F$	$(^3F)^4F$				
3.5	19	$(^1D)^2F$	$(^1G)^2F$	$(^3P)^2F$	$(^3F)^2F$	$(^3H)^2F$	$(^1D)^2G$	$(^1I)^2G$
		$(^3H)^2G$	$(^1I)^2G$	$(^3P)^4D$	$(^3F)^4D$	$(^3P)^4F$	$(^3F)^4F$	$(^3H)^4F$
		$(^3H)^4G$	$(^3F)^4H$	$(^3H)^4H$	$(^3F)^2G$	$(^3F)^4G$		
4.5	15	$(^1D)^2G$	$(^1I)^2G$	$(^3F)^2G$	$(^3H)^2G$	$(^1I)^2G$	$(^1I)^2H$	$(^3F)^2H$
		$(^3P)^4F$	$(^3F)^4F$	$(^3H)^4F$	$(^3F)^4G$	$(^3H)^4G$	$(^3F)^4H$	$(^3H)^4H$
		$(^3H)^2H$						
5.5	13	$(^1G)^2H$	$(^1I)^2H$	$(^3F)^2H$	$(^3H)^2H$	$(^1G)^2I$	$(^1I)^2I$	$(^3H)^2I$
		$(^3H)^4G$	$(^3F)^4H$	$(^3H)^4H$	$(^3H)^4I$	$(^3H)^4K$	$(^3F)^4G$	
6.6	8	$(^1I)^2I$	$(^3H)^2I$	$(^1I)^2K$	$(^3H)^2K$	$(^3F)^4H$	$(^3H)^4H$	$(^3H)^4I$
		$(^3H)^4K$						
7.5	5	$(^1I)^2K$	$(^3H)^2K$	$(^1I)^2L$	$(^3H)^4I$	$(^3H)^4K$		
8.5	2	$(^1I)^2L$	$(^3H)^4K$					

Table III. coefficient of fractional parentage of 2D term

$L_oS_o/L'S'$	1S	1D	1G	1I	3P	3F	3H
1S	0	0	0	0	0	0	0
1D	-0.23	0.11	-0.19	0	-0.35	0.88	0
1G	0	0	0	0	0	0	0
1I	0	0	0	0	0	0	0
3P	-0.37	-0.424	0.759	0	0.31	0	0
3F	0	0	0	0	0	0	0
3H	0	0	0	0	0	0	0

Table IV. coefficient of fractional parentage of 2F term

$L_oS_o/L'S'$	1D	1G	3P	3F
1D	-0.479	-0.56	-0.632	-0.300
3P	-0.48	-0.76	0.132	0.40
3F	-0.314	-0.496	0.53	-0.62

Table V. coefficient of fractional parentage of 2G term

$L_oS_o/L'S'$	1D	1G	3F
1D	-0.21	0.57	-0.79
1G	-0.57	-0.16	0.81
3F	-0.65	0.68	0.31

Description of the wavefunctions

The wavefunctions found for the configuration $4f^25d6s^2$ are given in table VI. One of the wavefunction is $|f^2ds^2, (^1D)^2G\rangle = 0.576|f^2ds^2, (^1G)^2G\rangle - 0.797|f^2ds^2, (^3F)^2G\rangle$. The left-hand side shows the wavefunction belongs to the configuration $4f^25d6s^2$ of Pr I. The term in bracket (1D) is the principal parent. The second term 2G is the combination of two terms having different parent 1G and 3F . The numerical value are coefficients are coefficients of fractional parentage. The term 2G is one of the final terms of the configuration.

Table VI: Coupled wave function of configuration $4f^25d6s^2$

$ f^2ds^2, (^1G)^2I\rangle = +1 f^2ds^2, (^1G)^2I\rangle$	1
$ f^2ds^2, (^1G)^2H\rangle = 0.316 f^2ds^2, (^1G)^2H\rangle - 0.94 f^2ds^2, (^3F)^2H\rangle$	2

$ f^2ds^2, (^3F)^2H\rangle = -0.94 f^2ds^2, (^1G)^2H\rangle + 0.316 f^2ds^2, (^3F)^2H\rangle$	3
$ f^2ds^2, (^1G)^2G\rangle = -0.16 f^2ds^2, (^1G)^2G\rangle + 0.815 f^2ds^2, (^3F)^2G\rangle - 0.56 f^2ds^2, (^1D)^2G\rangle$	4
$ f^2ds^2, (^3F)^2G\rangle = 0.63 f^2ds^2, (^1G)^2G\rangle + 0.316 f^2ds^2, (^3F)^2G\rangle - 0.65 f^2ds^2, (^1D)^2G\rangle$	5
$ f^2ds^2, (^1D)^2G\rangle = 0.576 f^2ds^2, (^1G)^2G\rangle - 0.797 f^2ds^2, (^3F)^2G\rangle - 0.219 f^2ds^2, (^1D)^2G\rangle$	6
$ f^2ds^2, (^3F)^2F\rangle = -0.496 f^2ds^2, (^1G)^2F\rangle - 0.62 f^2ds^2, (^3F)^2F\rangle + 0.53 f^2ds^2, (^3P)^2F\rangle - 0.314 f^2ds^2, (^1D)^2F\rangle$	7
$ f^2ds^2, (^1D)^2F\rangle = -0.56 f^2ds^2, (^1G)^2F\rangle - 0.300 f^2ds^2, (^3F)^2F\rangle + 0.60 f^2ds^2, (^3P)^2F\rangle - 0.479 f^2ds^2, (^1D)^2F\rangle$	8
$ f^2ds^2, (^3P)^2F\rangle = -0.76 f^2ds^2, (^1G)^2F\rangle + 0.40 f^2ds^2, (^3F)^2F\rangle - 0.48 f^2ds^2, (^1D)^2F\rangle + 0.135 f^2ds^2, (^3P)^2F\rangle$	9
$ f^2ds^2, (^1D)^2D\rangle = -0.19 f^2ds^2, (^1G)^2D\rangle + 0.88 f^2ds^2, (^3F)^2D\rangle + 0.11 f^2ds^2, (^1D)^2D\rangle - 0.34 f^2ds^2, (^3P)^2D\rangle - 0.23 f^2ds^2, (^1S)^2D\rangle$	10
$ f^2ds^2, (^3P)^2D\rangle = +0.75 f^2ds^2, (^1G)^2D\rangle - 0.24 f^2ds^2, (^1D)^2D\rangle + 0.31 f^2ds^2, (^3P)^2D\rangle - 0.37 f^2ds^2, (^1S)^2D\rangle$	11
$ f^2ds^2, (^1S)^2D\rangle = -0.452 f^2ds^2, (^1G)^2D\rangle - 0.690 f^2ds^2, (^3F)^2D\rangle - 0.337 f^2ds^2, (^1D)^2D\rangle - 0.452 f^2ds^2, (^3P)^2D\rangle - 0.14 f^2ds^2, (^1S)^2D\rangle$	12
$ f^2ds^2, (^1D)^2P\rangle = -0.66 f^2ds^2, (^3F)^2P\rangle + 0.5 f^2ds^2, (^1D)^2P\rangle + 0.648 f^2ds^2, (^3P)^2P\rangle$	13
$ f^2ds^2, (^3P)^2P\rangle = -0.56 f^2ds^2, (^3F)^2P\rangle + 0.785 f^2ds^2, (^1D)^2P\rangle - 0.22 f^2ds^2, (^3P)^2P\rangle$	14
$ f^2ds^2, (^1D)^2S\rangle = 1 f^2ds^2, (^1D)^2S\rangle$	15
$ f^2ds^2, (^3F)^4H\rangle = +1 f^2ds^2, (^3F)^4H\rangle$	16
$ f^2ds^2, (^3F)^4G\rangle = +1 f^2ds^2, (^3F)^4G\rangle$	17
$ f^2ds^2, (^3F)^4F\rangle = 0.76 f^2ds^2, (^3F)^4F\rangle - 0.65 f^2ds^2, (^3P)^4F\rangle$	18
$ f^2ds^2, (^3P)^4F\rangle = -0.95 f^2ds^2, (^3F)^4F\rangle - 0.317 f^2ds^2, (^3P)^4F\rangle$	19
$ f^2ds^2, (^3F)^4D\rangle = +1 f^2ds^2, (^3F)^4D\rangle$	20
$ f^2ds^2, (^3P)^4D\rangle = +1 f^2ds^2, (^3P)^4D\rangle$	21
$ f^2ds^2, (^3F)^4P\rangle = +0.25 f^2ds^2, (^3F)^4P\rangle + 0.97 f^2ds^2, (^3P)^4P\rangle$	22
$ f^2ds^2, (^3P)^4P\rangle = +0.929 f^2ds^2, (^3F)^4P\rangle + 0.37 f^2ds^2, (^3P)^4P\rangle$	23

Conclusion:-

In this paper we investigated configuration $4f^25d6s^2$ of Pr I to study fine level structure. The number of terms belong to this configuration are 42 (see table I), which results in 102 microstates. The J values of these 102 microstates and term symbols are given table II. The minimum value of J in configurations is 0.5 and the maximum value is 8.5. The coupled wave function of terms may have contribution of other terms of the configuration. The study also shows that there are 23 coupled wavefunction of the configuration $4f^25d6s^2$. These wavefunctions are given in equation (1) to (23), with corresponding cfp. The coefficient of fractional parentage gives idea of contribution of each of these terms. The results presented here are important as one use them in calculation of energies of the fine levels of Pr I belonging to configuration discussed above.

References:-

1. (Bransden et al., 2003) Bransden, B. H., Joachain, C. J., & Plivier, T. J. (2003). Physics of atoms and molecules. Pearson Education India.
2.)Condon et al., 1980) Condon et al. 1980 Condon, E. U., & Odabasi, H. (1980). Atomic structure. CUP Archive.
3.)Cowan, R.D, 1981) Cowan, R. D. (1981). The theory of atomic structure and spectra (No. 3). Univ of California Press.
4.)Furmann et al.,2006) Furmann, B., Krzykowski, A., Stefańska, D., & Dembczyński, J. (2006). New levels and hyperfine structure evaluation in neutral praseodymium. Physica Scripta, 74(6), 658
5.)Gamper et al., 2011) Gamper, B., Uddin, Z., Jahangir, M., Allard, O., Knöckel, H., Tiemann, E., & Windholz, L.
6.)Ginibre, A.,1981) Ginibre, A. (1981). Fine and hyperfine structures in the configurations 4f25d6s2 and 4f25d26s of neutral praseodymium. Physica Scripta, 23(3), 260.
7.)Ginibre, A.,1989) Ginibre, A. (1989). Fine and hyperfine structures of singly ionized praseodymium: I. energy levels, hyperfine structures and Zeeman effect, classified lines. Physica Scripta, 39(6), 694.
8.)Khan et al., 2016) Khan, S., Siddiqui, I., Iqbal, S. T., Uddin, Z., Guthöhrlein, G. H., & Windholz, L. (2016). Experimental investigation of the hyperfine structure of neutral praseodymium spectral lines and discovery of new energy levels. International Journal of Chemistry, 9(1), 7.
9.)Meena et al., 2013) Meena, P. L., Kumar, N., Meena, A. S., Meena, K. S., & Jain, P. K. (2013). Calculation of atomic spectroscopic terms for f 2 and f 12 orbital configurations, assigning the term symbols and comparative study. Bulgarian Chemical Communications, 45(3), 338-393.
10.)Murth, H.A et al., 2017) Murthy, H. A., & MRao, V. A Study on Atomic Spectroscopic Term Symbols for Non-equivalent Electrons of (n-1) d s p Configuration Using Russell-Saunders Coupling Scheme
11.)Racah, G. 1943) Racah, G. (1943). Theory of complex spectra. III. Physical Review, 63(9-10), 367.
12.)Siddiqi et al., 2014) Siddiqui I, Khan S and Windholz L 2014 Eur. Phys. J D
13.)Siddiqi et al., 2016) Siddiqui, I., Khan, S., & Windholz, L. (2016). Experimental investigation of the hyperfine spectra of Pr I-lines: discovery of new fine structure energy levels of Pr I using LIF spectroscopy with medium angular momentum quantum number between 7/2 and 13/2. The European Physical Journal D, 70(3), 44.
14.)Sobolewski et al., 2017) Sobolewski, Ł. M., Windholz, L., & Kwela, J. (2017). Laser induced fluorescence spectroscopy used for the investigation of Landé gJ-factors of praseodymium energy levels. Journal of Quantitative Spectroscopy and Radiative Transfer, 194, 24-30.
15.)Uddin, Z et al., 2012) Uddin, Z., Zafar, R., Sikander, R., Siddiqui, I., Shamim, K., & Windholz, L. (2012). Investigation of Pr I line by a simulation of their hyperfine patterns: discovery of new levels. Journal of Physics B: Atomic, Molecular and Optical Physics, 45(20), 205001.
16.)Uddin, Z 2014) Uddin, Z. (2014). New odd levels of Pr I with low angular momentum. Chinese Journal of Physics, 52(2), 770-779.
17.)Uddin, Z, 2015) Uddin, Z., Siddiqui, I., Tanweer, J., Jilani, S. U., & Windholz, L. (2015). Classification of some blended spectral lines of praseodymium. Journal of Physics B: Atomic, Molecular and Optical Physics, 48(13), 135001.
18. (W. C. Martin et al., 1978) W. C. Martin, R. Zalubas, and L. Hagan (1978), Atomic Energy Levels—The Rare Earth Elements National Bureau of Standards, vol. 60.