Wavefunctions for ground state $4f^3 6s^2$ configuration of praseodymium to calculate energy of fine levels and other spectroscopic quantities

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Abstract

Wave functions for terms with the same orbital angular momentum $L$ and spin angular momentum $S$, but different parents can be written as a linear combination of the pure parentage wave functions. These wavefunctions are important because various spectroscopic quantities e.g. energy and transition probability can be calculated with the help of these wavefunctions. In this study we present 46 wavefunctions of seventeen terms ($^2P$, $^2D$, $^2F$, $^2G$, $^2H$, $^2I$, $^2K$, $^2L$, $^4S$, $^4D$, $^4F$, $^4G$, $^4I$, $^4D$, $^2F$, $^2G$, $^2H$) are repeated terms, all terms have seniority number 3 except $^2F$ whose seniority number is 1) of $4f^3 6s^2$ configuration of Pr I, with seven parents ($^4S$, $^1D$, $^1G$, $^1I$, $^3P$, $^3F$, $^1H$) belonging to $f^2$. Some of the wavefunctions are non-orthogonal as they belong to same term symbol, having different seniority number. Gram-Schmidt procedure was used to make them orthogonal.

Introduction

Praseodymium ($^{141}$Pr) is a lanthanide group element, its electronic configuration is [Xe] $4f^3 6s^2$. It is a soft silvery-yellow metal. It forms Green Oxides (Pr$_2$O$_3$) with oxygen. To avoid corrosion, it is layered with oil or kept air tight. Naturally occurring Praseodymium has no other isotope. It occurs in the Earth’s crust and also abundant in stars. Its alloy with magnesium are mainly used in aircrafts engines due to their high metallic strength. Praseodymium constitutes about 5% of misch metals. It is also used as a core in carbon arc lights. In fiber optics it is used as a doping agent. One of its foremost applications lies in the construction of certain types of welder’s goggles.

Praseodymium is very rich in fine levels. Many Scientists studied the electronic configuration of Pr and published results on fine structure [1]. In 1981 A Ginibre studied hyper fine (hf) structure of praseodymium based on the analysis of high-resolution recordings lying in the IR (infrared) and visible ranges; she demonstrated the experimental energies of 54 levels of Pr atom [2]. Alongside she also studied the fine and hyperfine structure of singly ionized praseodymium ion (Pr II) by Fourier transform spectroscopy. Based on her high-resolution data lying in the range 2783–27920 cm$^{-1}$, she found new energy levels of the odd configuration $4f^2 5d^6p$ and of the mixed even configurations $4f^2 5d^2$, $4f^2 5d^5 6s$ and $4f^3 6p$ [3, 4]. In 1988 M N Reddy and G N Rao recorded the atomic spectra of Praseodymium atom using Laser Optogalvanic spectroscopy and recognized 78 atomic transition of neutral atom and 43 transition of singly ionized Pr atom (Pr II). They also reported hyperfine structure of few lines in neutral Praseodymium [5]. In 1997 A Krzykowski et al studied the hyperfine structure(hf) in the configuration $4f^3 5d 6s$ of Pr I and reported the hyperfine constant of the lower level belonging to this configuration by using laser induced florescence LIF technique [6]. In 2001 Furmann et al evaluate three new low-lying levels of Pr II and reported the hyperfine structure of some unclassified lines. They also measured hyperfine constant of some known levels more precisely and found consistent with previous literature data [7]. In 2002 M Hong liang studied hyperfine structure of singly ionized lanthanum and
Praseodymium by sing collinear fast ion beam laser spectrometer and reported the electric quadrupole (A) and magnetic dipole (B) constant [8]. In 2006 Furman et al investigated spectral lines of neutral praseodymium with the method of laser-induced fluorescence (LIF), leading to the discovery of 54 new hyperfine levels [9]. In 2011 Syed et al investigated the hyperfine structure of Pr by using LIF and founded 18 new levels of even parity and 22 of odd parity [10]. With the aid of Laser excitation and fluorescence observation further classified 246 lines of Pr.

In the same year Gamper et al recorded new highly resolved Fourier transformed spectrum of the praseodymium atom and found about 9000 new lines of Pr and categorize 1194 lines as transitions between energy levels of the Pr atom and 19 as transitions of the Pr ion. They also discovered twenty-three new atomic energy levels of odd parity and one of even parity [11]. In 2012, 2014 and 2015 Zaheer et al reported the discovery of new levels of Pr using LIF technique. In 2016 Siddiqui, Shamim and Windholz reported 32 new even parity and 38 odd parity levels of PrI [12–14]. In 2017 Sobolewski, Windholz and Kwpela investigated 52 lines of Pr I in the range of 516.3 nm to 613.9 nm again by using LIF method; they also reported lande g factor of 71 levels of Pr I [15]. In 2019 our group calculated and reported wavefunctions of 4f^5 6s^2 configuration of Pr II [16]. Both theoretical experimental studies are done to study fine structure and to calculate energy of fine levels of Pr I and Pr II, due to complex atomic structure still study is incomplete. We studied fine structure of Pr I for electronic configuration 4f^5 6s^2. It is an odd parity configuration. The orthonormalized wave function of ground state configuration of Pr I 4f^5 6s^2 are presented in this work.

**Methodology**

To calculate the coupled wavefunctions of configuration 4f^5 6s^2 of Pr I, coefficient of fractional parentage method is used. In this method one chooses a trail principal parents given by L_0 S_0 to calculate whether a given principle produces non-zero and independent coefficient of fractional parentage. These wavefunctions are given as follows [17]: These equation can be obtained with the help of Wigner–Eckart Theorem [18] and Racah [19–22]

\[
\langle \text{a}^n \text{b}^m; (S_0 L_0) \alpha \xi \text{SL} | \text{a}^n \text{b}^m; (S_0 L_0) \alpha \xi \text{SL} \rangle = (-1)^{M + L + S + \frac{1}{2}} [S_0, L_0]^{\frac{1}{2}} \times \sum_{L' S' \alpha'} [L', S']^{\frac{1}{2}} \left\{ \frac{11 L_0}{11 L'} \right\} \left\{ \frac{s s S_0}{s s S'} \right\} \langle \text{a}^n \text{b}^m \text{L}' S' \xi | \text{a}^n \text{b}^m ; (S_0 L_0) \alpha \xi \text{SL} \rangle
\]

(1)

Here a and b are orbitals, \( n, m \) are the number of equivalent electrons, term in braces are 6j symbol given by wigner, term \( [(L, S)] = (2L + 1)(2S + 1) \) and \( \langle \text{a}^n \text{b}^m \alpha \xi \text{SL} \rangle \) is the coefficient of fractional parentage. The wavefunction arises from configuration \( \text{a}^n \text{b}^m \) which is written as \( \langle \text{a}^n \text{b}^m; (S_0 L_0) \alpha \xi \text{SL} \rangle \). Here \( S_0, L_0 \) are principal parent spin and orbital angular momenta. \( S \) and \( L \) are the spin and orbital angular momenta of the final terms of the configuration. The final term wavefunction is a linear combination of wavefunctions \( \langle \text{a}^n \text{b}^m; (L' S') \xi \text{SL} \rangle \). The calculated wavefunction from equation (1) of the terms, are not necessarily anti-symmetric because the terms with \( (L' S') \) are involved. We eliminate such terms before using this equation. The symmetric wavefunctions are not included in the list of results generated by the program. Since \( 5^2 \) contribution is immaterial in construction of wavefunctions, therefore, the terms of \( 5^2 \) are taken as parent terms and then wavefunctions of the configurations \( 4f^5 6s^2 \) are calculated. The Russell–Sander technique was used to generate the term value of configuration [13]. Total terms generated by this configuration are seventeen given as \( ^2 \text{P}(3), ^2 \text{D}(3), ^2 \text{D}(3), ^2 \text{F}(1), ^2 \text{F}(3), ^2 \text{G}(3), ^2 \text{G}(3), ^2 \text{H}(3), ^2 \text{I}(3), ^2 \text{K}(3), ^2 \text{L}(3), ^2 \text{S}(3), ^2 \text{D}(3), ^2 \text{F}(3), ^2 \text{G}(3), ^2 \text{I}(3)). \)

There are seven parent terms of each configuration, each parent is taken as principal parent and the equation (1) is used to calculated coefficients of contributing term in the wave function. Further details can be found in [17, 23]. The wave functions were normalized and their orthogonality was checked. In the case of non-orthogonal wave functions, Gram–Schmidt procedure of orthogonality was used.

**Results and discussion**

In the 4f^5 6s^2 configuration, S orbital is filled. Hence it does not contribute to the final terms. Hence method of generating terms for equivalent electrons was used to find the final terms of this configuration. A total of seventeen terms are generated for the configuration 4f^5 6s^2. Four \( ^2 \text{D}, ^2 \text{F}, ^2 \text{G} \) and \( ^2 \text{H} \) of the final terms occur twice. To find the wavefunctions of this configuration, \( ^2 \text{F} \) was used as parent configuration, which generated seven parent terms. The choice of seven terms as principal parents gives the coefficients of fractional parentage for 46 states of 4f^5 6s^2 configuration. Four of the final terms are repeated, hence their wavefunctions are non-orthogonal. To make them orthogonal, Gram Schmidt procedure is used. The coefficient of fractional parentage of term \( ^2 \text{F} \) and \( ^2 \text{H} \) are given in tables 1 and 2, respectively. It is observed that the choice of some terms as
principal parents has zero coefficient of fractional. The calculated wavefunctions are orthonormalized and are given in equations (3)–(48).

**Description of the wavefunctions**

The wavefunctions found for the configuration 4f36s2 are given below. One of the wavefunctions \( |f^3s^2, \langle I \rangle^2 L = 0.70 |f^3s^2, \langle I \rangle^2 L - 0.70 |f^3s^2, \langle H \rangle^2 L \). The left-hand side shows the wavefunction belonging to the ground state configuration 4f36s2 of Pr I. The term in bracket \( \langle I \rangle \) is the principal parent.

The second term is the combination of two terms having different parents \( 1^I \) and \( 3^H \). The numerical value are coefficients of fractional parentage. The term \( ^L \) is one of the final terms of the configuration.

**Coupled wave function of configuration \( f^3s^2 \)**

\[
|f^3s^2, (S)F = 0.535|f^3s^2, (S)F - 0.199|f^3s^2, (D)F - 0.275|f^3s^2, (G)F - 0.32
\]

\[
|f^3s^2, (D)F = -0.212|f^3s^2, (S)F + 0.515|f^3s^2, (D)F + 0.319|f^3s^2, (G)F - 0.478|f^3s^2, (P)F + 0.162|f^3s^2, (P)F + 0.509|f^3s^2, (H)F \tag{3}
\]

\[
|f^3s^2, (G)F = -0.217|f^3s^2, (S)F + 0.278|f^3s^2, (D)F + 0.185|f^3s^2, (G)F - 0.050|f^3s^2, (I)F - 0.154|f^3s^2, (P)F - 0.834|f^3s^2, (I)F + 0.342|f^3s^2, (H)F \tag{4}
\]

\[
|f^3s^2, (I)F = -0.005|f^3s^2, (S)F + 0.208|f^3s^2, (D)F - 0.872|f^3s^2, (G)F - 0.147|f^3s^2, (I)F + 0.168|f^3s^2, (P)F + 0.011|f^3s^2, (I)F + 0.381|f^3s^2, (H)F \tag{5}
\]

\[
|f^3s^2, (P)F = 0.218|f^3s^2, (S)F + 0.664|f^3s^2, (D)F - 0.105|f^3s^2, (G)F + 0.622|f^3s^2, (I)F - 0.165|f^3s^2, (P)F + 0.015|f^3s^2, (I)F - 0.290|f^3s^2, (H)F \tag{6}
\]

\[
|f^3s^2, (I)F = -0.284|f^3s^2, (S)F - 0.453|f^3s^2, (D)F - 0.258|f^3s^2, (G)F + 0.410|f^3s^2, (I)F - 0.68|f^3s^2, (P)F + 0.011|f^3s^2, (I)F + 0.108|f^3s^2, (H)F \tag{7}
\]

\[
|f^3s^2, (H)F = 7.271e - 01|f^3s^2, (S)F - 1.93e - 01|f^3s^2, (D)F + 1.618e - 01|f^3s^2, (G)F + 2.60e - 01|f^3s^2, (I)F + 1.724e - 02|f^3s^2, (P)F - 7.20e - 04|f^3s^2, (I)F + 5.80e - 01|f^3s^2, (H)F \tag{8}
\]

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**Table 1. Coefficient of fractional parentage of \( ^7F \) Term.**

| \( L_sS_l/L^0s^0 \) | \(^1S\) | \(^1D\) | \(^1G\) | \(^1I\) | \(^1P\) | \(^1F\) | \(^1H\) |
|---|---|---|---|---|---|---|---|
| \(^1S\) | 0.534 | -0.198 | -0.275 | -0.320 | -0.266 | -0.407 | -0.509 |
| \(^1D\) | 0.598 | 0.389 | 0.156 | -0.50 | -0.619 | 0.369 | 0.209 |
| \(^1G\) | -0.217 | 0.278 | 0.183 | -0.050 | -0.154 | -0.834 | 0.342 |
| \(^1I\) | -0.205 | 0.208 | -0.872 | -0.147 | 0.164 | 0.011 | 0.381 |
| \(^1P\) | 0.218 | 0.664 | -0.105 | 0.662 | -0.165 | 0.158 | -0.290 |
| \(^1F\) | -0.284 | -0.453 | -0.257 | 0.410 | -0.683 | 0.011 | 0.108 |
| \(^1H\) | 7.6e-01 | -2e-01 | 1.6e-01 | 2.6e-01 | 1.7e-02 | -7e-04 | 5e-01 |

**Table 2. Coefficient of fractional parentage of \( ^3H \) Term.**

| \( L_sS_l/L^0s^0 \) | \(^1D\) | \(^1G\) | \(^1I\) | \(^1F\) | \(^3H\) |
|---|---|---|---|---|---|
| \(^1D\) | 0.54 | -0.28 | -0.35 | -0.30 | -0.64 |
| \(^1G\) | 0.20 | 0.72 | -0.60 | 0.237 | 0.08 |
| \(^1I\) | 0.14 | -0.18 | 0.14 | 0.910 | -0.30 |
| \(^1F\) | 0.04 | 0.60 | 0.61 | -0.151 | -0.48 |
| \(^3H\) | -0.79 | 0.002 | -0.33 | 0.010 | -0.49 |
\[ f^3 s^2, (J^2 H) = +0.54[f^3 s^2, (J^2 H) - 0.28|f^3 s^2, (G)^2 H] - 0.35|f^3 s^2, (I)^2 H) - 0.30|f^3 s^2, (F)^2 H) - 0.642|f^3 s^2, (H)^2 H) \] (10)

\[ f^3 s^2, (G)^2 H) = -0.20|f^3 s^2, (J^2 H) + 0.72|f^3 s^2, (G)^2 H) - 0.60|f^3 s^2, (I)^2 H) - 0.23|f^3 s^2, (F)^2 H) + 0.080|f^3 s^2, (H)^2 H) \] (11)

\[ f^3 s^2, (J)^2 H) = -0.141|f^3 s^2, (J^2 H) - 0.182|f^3 s^2, (G)^2 H) + 0.147|f^3 s^2, (I)^2 H) + 0.910|f^3 s^2, (F)^2 H) - 0.308|f^3 s^2, (H)^2 H) \] (12)

\[ f^3 s^2, (F)^2 H) = 0.040|f^3 s^2, (D)^2 H) + 0.602|f^3 s^2, (G)^2 H) + 0.611|f^3 s^2, (I)^2 H) - 0.151|f^3 s^2, (F)^2 H) - 0.48|f^3 s^2, (H)^2 H) \] (13)

\[ f^3 s^2, (H)^2 H) = -0.799|f^3 s^2, (D)^2 H) + 0.002|f^3 s^2, (G)^2 H) - 0.335|f^3 s^2, (I)^2 H) + 0.0106|f^3 s^2, (F)^2 H) - 0.497|f^3 s^2, (H)^2 H) \] (14)

\[ f^3 s^2, (D)^2 P) = +0.489|f^3 s^2, (D)^2 P) - 0.513|f^3 s^2, (G)^2 P) - 0.708|f^3 s^2, (F)^2 P) \] (15)

\[ f^3 s^2, (G)^2 P) = -0.483|f^3 s^2, (D)^2 P) + 0.506|f^3 s^2, (G)^2 P) + 0.7|f^3 s^2, (F)^2 P) \] (16)

\[ f^3 s^2, (F)^2 P) = -0.49|f^3 s^2, (D)^2 P) + 0.51|f^3 s^2, (G)^2 P) + 0.71|f^3 s^2, (F)^2 P) \] (17)

\[ f^3 s^2, (D)^2 D) = +0.71|f^3 s^2, (D)^2 D) + 0.24|f^3 s^2, (P)^2 D) \]
\[ + 0.35|f^3 s^2, (F)^2 D) - 0.553|f^3 s^2, (H)^2 D) \] (18)

\[ f^3 s^2, (G)^2 D) = +0.71|f^3 s^2, (G)^2 D) + 0.476|f^3 s^2, (P)^2 D) \]
\[ - 0.514|f^3 s^2, (F)^2 D) - 0.117|f^3 s^2, (H)^2 D) \] (19)

\[ f^3 s^2, (P)^2 D) = +0.327|f^3 s^2, (D)^2 D) + 0.628|f^3 s^2, (G)^2 D) \]
\[ + 0.535|f^3 s^2, (P)^2 D) - 0.288|f^3 s^2, (F)^2 D) - 0.362|f^3 s^2, (H)^2 D) \] (20)

\[ f^3 s^2, (F)^2 D) = +0.405|f^3 s^2, (D)^2 D) - 0.58|f^3 s^2, (G)^2 D) \]
\[ - 0.24|f^3 s^2, (P)^2 D) + 0.626|f^3 s^2, (F)^2 D) - 0.224|f^3 s^2, (H)^2 D) \] (21)

\[ f^3 s^2, (H)^2 D) = -0.696|f^3 s^2, (D)^2 D) - 0.145|f^3 s^2, (G)^2 D) \]
\[ - 0.34|f^3 s^2, (P)^2 D) - 0.245|f^3 s^2, (F)^2 D) - 0.57|f^3 s^2, (H)^2 D) \] (22)

\[ f^3 s^2, (D)^2 G) = +0.43|f^3 s^2, (D)^2 G) - 0.21|f^3 s^2, (G)^2 G) + 0.50|f^3 s^2, (I)^2 G) \]
\[ - 0.3|f^3 s^2, (P)^2 G) - 0.61|f^3 s^2, (F)^2 G) + 0.18|f^3 s^2, (H)^2 G) \] (23)

\[ f^3 s^2, (G)^2 G) = -4.47 e - 04|f^3 s^2, (D)^2 G) + 6.50 e - 01|f^3 s^2, (G)^2 G) \]
\[ + 2.77 e - 01|f^3 s^2, (I)^2 G) - 5.26 e - 01|f^3 s^2, (P)^2 G) + 1.21 e - 01|f^3 s^2, (F)^2 G) \]
\[ - 4.56 e - 01|f^3 s^2, (H)^2 G) \] (24)

\[ f^3 s^2, (I)^2 G) = -0.11|f^3 s^2, (D)^2 G) + 0.34|f^3 s^2, (G)^2 G) \]
\[ + 0.07|f^3 s^2, (I)^2 G) - 0.23|f^3 s^2, (P)^2 G) + 0.23|f^3 s^2, (F)^2 G) |f^3 s^2, (H)^2 G) \] (25)

\[ f^3 s^2, (P)^2 G) = +0.89|f^3 s^2, (D)^2 G) + 14|f^3 s^2, (G)^2 G) \]
\[ - 0.26|f^3 s^2, (I)^2 G) + 0.09|f^3 s^2, (P)^2 G) + 0.33|f^3 s^2, (F)^2 G) + 0.02|f^3 s^2, (H)^2 G) \] (26)

\[ f^3 s^2, (F)^2 G) = -0.025|f^3 s^2, (D)^2 G) - 0.56|f^3 s^2, (G)^2 G) \]
\[ - 0.24|f^3 s^2, (I)^2 G) - 0.71|f^3 s^2, (P)^2 G) + 0.32|f^3 s^2, (F)^2 G) - 0.04|f^3 s^2, (H)^2 G) \] (27)

\[ f^3 s^2, (H)^2 G) = 0.01|f^3 s^2, (D)^2 G) - 0.26|f^3 s^2, (G)^2 G) + 0.72|f^3 s^2, (I)^2 G) \]
\[ + 0.23|f^3 s^2, (P)^2 G) + 0.58|f^3 s^2, (F)^2 G) - 0.05|f^3 s^2, (H)^2 G) \] (28)
\begin{align*}
|f^3s^2, (\bar{G}G)^2I\rangle &= +0.37|f^3s^2, (\bar{G}G)^2I\rangle + 0.60|f^3s^2, (\bar{I}I)^2I\rangle \\
& - 0.62|f^3s^2, (\bar{F}F)^2I\rangle - 0.33|f^3s^2, (\bar{H}H)^2I\rangle
\end{align*}
(29)

\begin{align*}
|f^3s^2, (\bar{I}I)^2I\rangle &= 0.37|f^3s^2, (\bar{G}G)^2I\rangle + 0.60|f^3s^2, (\bar{I}I)^2I\rangle \\
& - 0.71|f^3s^2, (\bar{F}F)^2I\rangle - 0.33|f^3s^2, (\bar{H}H)^2I\rangle
\end{align*}
(30)

\begin{align*}
|f^3s^2, (\bar{F}F)^2I\rangle &= -0.37|f^3s^2, (\bar{G}G)^2I\rangle - 0.60|f^3s^2, (\bar{I}I)^2I\rangle \\
& + 0.62|f^3s^2, (\bar{F}F)^2I\rangle + 0.33|f^3s^2, (\bar{H}H)^2I\rangle
\end{align*}
(31)

\begin{align*}
|f^3s^2, (\bar{H}H)^2I\rangle &= -0.37|f^3s^2, (\bar{G}G)^2I\rangle - 0.60|f^3s^2, (\bar{I}I)^2I\rangle \\
& + 0.62|f^3s^2, (\bar{F}F)^2I\rangle + 0.33|f^3s^2, (\bar{H}H)^2I\rangle
\end{align*}
(32)

\begin{align*}
|f^3s^2, (\bar{G}G)^2K\rangle &= 0.49|f^3s^2, (\bar{G}G)^2K\rangle - 0.50|f^3s^2, (\bar{I}I)^2K\rangle - 0.71|f^3s^2, (\bar{H}H)^2K\rangle
\end{align*}
(33)

\begin{align*}
|f^3s^2, (\bar{I}I)^2K\rangle &= -0.49|f^3s^2, (\bar{G}G)^2K\rangle + 0.50|f^3s^2, (\bar{I}I)^2K\rangle + 0.707|f^3s^2, (\bar{H}H)^2K\rangle
\end{align*}
(34)

\begin{align*}
|f^3s^2, (\bar{H}H)^2K\rangle &= -0.49|f^3s^2, (\bar{G}G)^2K\rangle + 0.50|f^3s^2, (\bar{I}I)^2K\rangle + 0.707|f^3s^2, (\bar{H}H)^2K\rangle
\end{align*}
(35)

\begin{align*}
|f^3s^2, (\bar{I}I)^2L\rangle &= 0.70|f^3s^2, (\bar{I}I)^2L\rangle - 0.70|f^3s^2, (\bar{H}H)^2L\rangle
\end{align*}
(36)

\begin{align*}
|f^3s^2, (\bar{H}H)^2L\rangle &= 0.70|f^3s^2, (\bar{I}I)^2L\rangle - 0.70|f^3s^2, (\bar{H}H)^2L\rangle
\end{align*}
(37)

\begin{align*}
|f^3s^2, (\bar{P})^4D\rangle &= +0.65|f^3s^2, (\bar{P})^4D\rangle + 0.471|f^3s^2, (\bar{F}F)^4D\rangle + 0.591|f^3s^2, (\bar{H}H)^4D\rangle
\end{align*}
(38)

\begin{align*}
|f^3s^2, (\bar{F}F)^4D\rangle &= +0.656|f^3s^2, (\bar{P})^4D\rangle + 0.472|f^3s^2, (\bar{F}F)^4D\rangle + 0.592|f^3s^2, (\bar{H}H)^4D\rangle
\end{align*}
(39)

\begin{align*}
|f^3s^2, (\bar{F})^4D\rangle &= +0.665|f^3s^2, (\bar{P})^4D\rangle + 0.471|f^3s^2, (\bar{F}F)^4D\rangle + 0.591|f^3s^2, (\bar{H}H)^4D\rangle
\end{align*}
(40)

\begin{align*}
|f^3s^2, (\bar{P})^4F\rangle &= 0.261|f^3s^2, (\bar{P})^4F\rangle - 0.817|f^3s^2, (\bar{F}F)^4F\rangle + 0.513|f^3s^2, (\bar{H}H)^4F\rangle
\end{align*}
(41)

\begin{align*}
|f^3s^2, (\bar{F}F)^4F\rangle &= -0.26|f^3s^2, (\bar{P})^4F\rangle + 0.81|f^3s^2, (\bar{F}F)^4F\rangle - 0.52|f^3s^2, (\bar{H}H)^4F\rangle
\end{align*}
(42)

\begin{align*}
|f^3s^2, (\bar{H}H)^4F\rangle &= 0.261|f^3s^2, (\bar{P})^4F\rangle - 0.817|f^3s^2, (\bar{F}F)^4F\rangle + 0.513|f^3s^2, (\bar{H}H)^4F\rangle
\end{align*}
(43)

\begin{align*}
|f^3s^2, (\bar{P})^4G\rangle &= +0.53|f^3s^2, (\bar{P})^4G\rangle - 0.49|f^3s^2, (\bar{F}F)^4G\rangle - 0.69|f^3s^2, (\bar{H}H)^4G\rangle
\end{align*}
(44)

\begin{align*}
|f^3s^2, (\bar{F}F)^4G\rangle &= -0.51|f^3s^2, (\bar{P})^4G\rangle + 0.47|f^3s^2, (\bar{F}F)^4G\rangle + 0.71|f^3s^2, (\bar{H}H)^4G\rangle
\end{align*}
(45)

\begin{align*}
|f^3s^2, (\bar{H}H)^4G\rangle &= -0.51|f^3s^2, (\bar{P})^4G\rangle + 0.47|f^3s^2, (\bar{F}F)^4G\rangle + 0.71|f^3s^2, (\bar{H}H)^4G\rangle
\end{align*}
(46)

\begin{align*}
|f^3s^2, (\bar{F})^4H\rangle &= +0.47|f^3s^2, (\bar{F})^4H\rangle - 0.88|f^3s^2, (\bar{H}H)^4I\rangle
\end{align*}
(47)

\begin{align*}
|f^3s^2, (\bar{H}H)^4I\rangle &= -0.47|f^3s^2, (\bar{F})^4H\rangle + 0.88|f^3s^2, (\bar{H}H)^4I\rangle
\end{align*}
(48)

**Conclusion**

To summarize, in this work forty six orthonormal wavefunctions of odd parity configuration $4f^36s^2$ of Pr I are reported, with their coefficients of fractional parentage. Due to the repetition of four terms, wave functions were not orthogonal; they were orthogonalized by Gram-Schmidt technique. In tables 1 and 2, coefficients of fractional parentage of term $^2F$ and $^2H$ are given with respect to their parents. These wavefunctions are important for theoretical calculations of energies of fine levels of the configuration $4f^36s^2$.

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