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RESEARCH ARTICLE

COULOMB ENERGIES FOR THE CONFIGURATION $4f^25d^2$ AND FINE LEVEL DETAILS OF THE CONFIGURATIONS $4f^36p$ & $4f^36s$ OF SINGLY IONIZED PRASEODYMIUM (PR II).

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Abstract

Pr II is first ion of atomic Praseodymium (Pr) (rare Earth element with $Z = 59$). In this study, we investigated electronic configurations $4f^36p$ & $4f^36s$ of singly ionized Praseodymium and studied its fine levels structure. We used Russell Saunders technique to calculate spectral terms, total angular momentum. The possible spectroscopic terms for (i) $4f^36p$ (ii) $4f^36s$ configurations are 98 and 34, respectively. The total number of J values corresponding to these configurations is 242 and 82, respectively. In addition, we investigated configuration $4f^25d^2$ and also found term energies arising from coulomb interaction. The total number of spectroscopic LS terms for $4f^25d^2$ are 187, Coulomb energies have also been calculated for these spectroscopic terms. The information presented in this paper could be further used to find other spectroscopic characteristics of the configurations.

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Introduction:-

Praseodymium (Pr), having atomic number (Z) = 59, is one of the elements from lanthanide series. It is a soft, silver and ductile metal. At any temperature above 1 K, Pr shows paramagnetic behavior unlike the other rare earth elements which behave ferromagnetic or anti ferromagnetic at low temperatures. Pr ¹⁴¹ is the only stable isotope with nuclear spin $I = 5/2$. Singly ionized praseodymium (Pr II) which is the first ion of Pr has very rich and complex optical spectrum because of its open 4f shell. For many years Pr alloys have been used in lightning engineering like in energy-saving lamps, fluorescence tubes, glasses and catalysts. Its spectral lines are also included in the stellar spectrum (Kurucz, 1993). It is also used as doping material in fluoride glass to increase the strength of optical fiber (Jha et al., 1995). Initially King and White studied fine and hyper fine structure of Pr I and Pr II (King, 1928; White 1929). H. Lew measured total angular momentum, nuclear spin, g J values and used Russell Saunder scheme and Hund's rule to determine ground state of neutral Pr for $4f^36s^2$ configuration and found $^4I_{3/2}$ to be ground state term (Lew, 1953). Experimental and theoretical investigations regarding fine and hyperfine structure of Pr I and Pr II spectral line were performed by many scientists and revealed lots of new levels for different configurations (Ginibre, 1989; Ruczkowski et al., 2003; Furmann et al., 2005; Furmann et al. 2006; Gamper et al., 2011). Hyperfine pattern of Pr atom through Fourier transform spectrum was studied and new energy levels of Pr atom were discovered (Zaheer et al., 2012). 54 spectral lines of Pr II was investigated by using high resolution spectroscopic method of collinear laser ion beam spectroscopy (CLIBS) and magnetic dipole interaction constants A and electric quadrupole interaction constant B of 49 involved levels were also found (Akhtar et al., 2012). Werbowy et al. used same technique to study Zeeman effect of Pr II spectral lines at low magnetic field up to 330 G. They measured

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Zeeman hyperfine structure patterns with visibly resolved components and Lande g J factors were also found for 39 Pr II levels of $4f^35d$, $4f^25d^2$ and $4f^36p$ configurations (Werbowsy et al., 2014). In 2017 Werbowsy et al. found Lande g J factor of 14 levels of f^3d odd and 16 levels of f^3p and f^2d^2 even configurations from 570.45 to 609.038 nm ranges and compared experimental values of Lande factors from previous measurements and with theoretical calculations (Werbowsy et al., 2017). Term values give information about spectral and magnetic properties of an element and used to find spin multiplicity, total angular momentum and energy of any atomic state. For f^3 and f^{11} equivalent electronic configuration, total 364 microstates and 17 allowed spectroscopic terms were determined (Meena et.al, 2012) and 91 possible microstates and 7 allowed term values were calculated for f^2 and f^{12} equivalent electronic configuration (Meena et.al, 2013).

The objective of this work is to calculate spectroscopic allowed term values, total angular momentum of fine levels for (i) $4f^36p$ (ii) $4f^36s$ configurations and term energies for (iii) $4f^25d^2$ of Pr II by using Russell Saunder coupling and coulomb interaction energy expression.

Methodology:-

Atomic spectroscopic terms and fine levels for electronic configurations were found by using Russell- Saunders coupling technique. Term values are represented by $^{(2S+1)}L_J$, where $2S+1$ is the spin multiplicity which refers to singlet, doublet, triplet terms and so on, S is total spin quantum number, can be calculated by vector addition of all spin quantum number, L is total orbital quantum number which is formed by vector addition of all orbital angular quantum number, J is the total angular quantum number which is vector sum of L and S. J values are given by $(L + S), (L + S) - 1, |L - S|$. The stability order and ground state term for given configuration can be determined by using Hund's rule scheme, which is

- Highest spin multiplicity indicates the lowest energy term.
- For same multiplicity terms, the lowest energy term is that which has larger value of orbital angular momentum.
- If sub shell is filled more than half, larger value of J has minimum energy.
- If sub shell is filled less than half, lowest J value corresponds to minimum energy.

The terms are determined by considering equivalent and non-equivalent electrons, for example, in configuration $4f^36p$, the terms arising from equivalent electron f^3 are found first by taking Pauli's principle into account. Combination rule was applied to find allowed terms. In next step terms were generated by adding a 'p' electron of 6th shell. Total 98 terms and 242 fine levels were generated by $4f^36p$ configuration (Sobel'man, 1967).

To express the Coulomb interaction energy $W(a,b; S,L)$ energy arising from coulomb interaction are calculated. It depends on $F^k(a,b)$ and $G^k(a,b)$ radial integrals as given in equation (A), where a, b are orbital quantum number of $4f^25d^2$. For final expression of term energy E (a, b, S, L) average energy of an electron pair is added to $W(a,b; S,L)$ see equation (B) (Condon & Odabasi, 1980).

$$W(a, b; S, L) = (2l_a + 1)(2l_b + 1) \left[(-1)^L \sum_k \begin{Bmatrix} l_a & l_b & L \\ l_b & l_a & k \end{Bmatrix} \begin{pmatrix} l_a & l_a & k \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_b & l_b & k \\ 0 & 0 & 0 \end{pmatrix} F^k(a, b) + (-1)^S \sum_k \begin{Bmatrix} l_a & l_b & L \\ l_a & l_b & k \end{Bmatrix} \begin{pmatrix} l_a & l_b & k \\ 0 & 0 & 0 \end{pmatrix}^2 G^k(a, b) \right] \quad (A)$$

$$E(a, b; S, L) = W(a, b; S, L) - F^0(a, b) + \frac{1}{2} \sum_k \begin{pmatrix} l_a & l_b & k \\ 0 & 0 & 0 \end{pmatrix}^2 G^k(a, b) \quad (B)$$

Results and Discussion:-

Three electronic configurations (i) $4f^36p$ (ii) $4f^36s$ (iii) $4f^25d^2$ were investigated for fine structure detail of Pr II. Total number of atomic spectroscopic terms calculated for (i) $4f^36p$ (ii) $4f^36s$ configurations are 98 and 34 respectively. Hund's rule was used to determine stability order and ground state of configuration. In $4f^36p$ configuration out of 98 terms, 7 types are quintets, 10 types are triplets, and 10 types are singlets. The stability order term is $^5K > ^5I > ^5H > ^5G > ^5F > ^5D > ^5P > ^3M > ^3L > ^3K > ^3I > ^3H > ^3G > ^3F > ^3D > ^3P > ^3S > ^1M > ^1L > ^1K > ^1I > ^1H > ^1G > ^1F > ^1D > ^1P > ^1S$. For electronic configuration $4f^36s$ out of 34 terms, 5 types are quintet, 9 types are triplet and 8 types are singlet. The stability array for this configuration is $^5I > ^5G > ^5F > ^5D > ^5S > ^3L > ^3K > ^3I > ^3H > ^3G > ^3F > ^3D > ^3P > ^3S > ^1L > ^1K > ^1I > ^1H > ^1G > ^1F > ^1D > ^1P$. Tables I and III shows allowed term

values with their frequency for (i) $4f^36p$ (ii) $4f^36s$ configurations respectively. In table II and IV details of fine levels are given. In first column total angular momentum is given, in second column the frequency of occurrence of J is given, the third column shows the terms generated by corresponding configuration, and in the last column the parent terms are given.

(i)The Configuration $4f^36p$.

The configuration $4f^36p$ generates 98 atomic spectroscopic LS terms and total fine levels corresponding to different J values are 242. Number of levels with J=3 have maximum frequency. Ground state term for this configuration is quintet K (5K) and it is further split up into five energy states i.e. $^5K_5, ^5K_6, ^5K_7, ^5K_8$ and 5K_9 because of orbit- spin interaction coupling. Different LS term values with the number of terms occurring in this configuration are given in Table I. J values lie between $0 \leq J \leq 10$ and frequencies of each J are given in Table II.

(ii) The Configuration $4f^36s$.

The configuration $4f^36s$ contains 34 LS term values and total fine levels corresponding to different J values are 82. Levels with J=3 and J=4 have highest frequency and ground state term is 5I which is further divided into five energy states $^5I_4, ^5I_5, ^5I_6, ^5I_7$ and 5I_8 . Different LS term values with their quantities are given in Table III. J values range between $0 \leq J \leq 9$ with frequencies are given in Table IV.

(ii) The Configuration $4f^25d^2$.

There are total 187 term values for $4f^25d^2$ configuration and total 181 term energies corresponding to resultant term are calculated and six terms contribute nothing in term energy and given in Table V. We have already found its terms values and corresponding wavefunctions of this configuration (submitted for publication). In this paper we present the coulomb interaction energies of 187 levels of configuration $4f^25d^2$, these energies are given in equations (1) to (181).

Conclusion:-

We studied fine structure of Pr II for three of its electronic configurations, namely (i) $4f^36p$ (ii) $4f^36s$ (iii) $4f^25d^2$. Coupling of angular momenta is carried out using Russell-Saunders method. The numbers of terms generated by these configurations are 98, 34 and 187, respectively. There are a total number of 781 fine levels belonging to the configurations under study. The numbers of levels corresponding to each of these configurations are 242, 82, and 457, respectively. For configuration $4f^25d^2$ coulomb interaction energies are calculated for 187 terms of the configuration. These energies can be further used with the spin-orbit energies to calculate center of gravity wavenumber of fine levels.

Table I:- Allowed LS Term Values of $4f^36p$.

Terms	1S	1P	1D	1F	1G	1H	1I	1K	1L	1M
Quantity	1	3	5	6	6	5	4	3	2	1
Terms	3S	3P	3D	3F	3G	3H	3I	3K	3L	3M
Quantity	1	5	7	9	8	7	5	4	2	1
Terms	-----	5P	5D	5F	5G	5H	5I	5K	-----	-----
Quantity	-----	2	2	3	2	2	1	1	-----	-----

Table II:- Designation of Fine levels corresponds to $4f^36p$.

J	Frequency	Terms				
0	8	$^1S(^2P+^2P)$	$^3P(^2P+^2P)$	$^3P(^2P+^2D)$	$^3P(^2P+^2D)$	$^3P(^2P+^4S)$
		$^3P(^2P+^4D)$	$^5D(^2P+^4D)$	$^5D(^2P+^4F)$		
1	23	$^1P(^2P+^2P)$	$^1P(^2P+^2D)$	$^1P(^2P+^2D)$	$^3S(^2P+^2P)$	$^3P(^2P+^2P)$
		$^3P(^2P+^2D)$	$^3P(^2P+^2D)$	$^3P(^2P+^4S)$	$^3P(^2P+^4D)$	$^5P(^2P+^4S)$
		$^5P(^2P+^4D)$	$^3D(^2P+^2P)$	$^3D(^2P+^2D)$	$^3D(^2P+^2D)$	$^3D(^2P+^2F)$
		$^3D(^2P+^2F)$	$^3D(^2P+^4D)$	$^3D(^2P+^4F)$	$^5D(^2P+^4D)$	$^5D(^2P+^4F)$
		$^5F(^2P+^4G)$	$^5F(^2P+^4F)$	$^5F(^2P+^4D)$		
2	35	$^1D(^2P+^2P)$	$^1D(^2P+^2D)$	$^1D(^2P+^2D)$	$^1D(^2P+^2F)$	$^1D(^2P+^2F)$
		$^3P(^2P+^2P)$	$^3P(^2P+^2D)$	$^3P(^2P+^2D)$	$^3P(^2P+^4S)$	$^3P(^2P+^4D)$
		$^3D(^2P+^2P)$	$^3D(^2P+^2D)$	$^3D(^2P+^2D)$	$^3D(^2P+^2F)$	$^3D(^2P+^2F)$
		$^3D(^2P+^4D)$	$^3D(^2P+^4F)$	$^3F(^2P+^2F)$	$^3F(^2P+^2F)$	$^3F(^2P+^2D)$

		$^3F(^2P+^2D)$	$^3F(^2P+^2G)$	$^3F(^2P+^2G)$	$^3F(^2P+^4D)$	$^3F(^2P+^4F)$
		$^3F(^2P+^4G)$	$^5P(^2P+^4S)$	$^5P(^2P+^4D)$	$^5D(^2P+^4D)$	$^5D(^2P+^4F)$
		$^5F(^2P+^4D)$	$^5F(^2P+^4F)$	$^5F(^2P+^4G)$	$^5G(^2P+^4F)$	$^5G(^2P+^4G)$
3	41	$^3D(^2P+^2P)$	$^3D(^2P+^2D)$	$^3D(^2P+^2D)$	$^3D(^2P+^2F)$	$^3D(^2P+^2F)$
		$^3D(^2P+^4D)$	$^3D(^2P+^4F)$	$^1F(^2P+^2D)$	$^1F(^2P+^2D)$	$^1F(^2P+^2F)$
		$^1F(^2P+^2F)$	$^1F(^2P+^2G)$	$^1F(^2P+^2G)$	$^3F(^2P+^2D)$	$^3F(^2P+^2D)$
		$^3F(^2P+^2F)$	$^3F(^2P+^2F)$	$^3F(^2P+^2G)$	$^3F(^2P+^2G)$	$^3F(^2P+^4D)$
		$^3F(^2P+^4F)$	$^3F(^2P+^4G)$	$^3G(^2P+^2F)$	$^3G(^2P+^2F)$	$^3G(^2P+^2G)$
		$^3G(^2P+^2G)$	$^3G(^2P+^2H)$	$^3G(^2P+^2H)$	$^3G(^2P+^4F)$	$^3G(^2P+^4G)$
		$^5G(^2P+^4F)$	$^5G(^2P+^4G)$	$^5P(^2P+^4S)$	$^5P(^2P+^4D)$	$^5D(^2P+^4D)$
		$^5D(^2P+^4F)$	$^5F(^2P+^4D)$	$^5F(^2P+^4F)$	$^5F(^2P+^4G)$	$^5H(^2P+^4G)$
		$^5H(^2P+^4I)$				
4	40	$^1G(^2P+^2H)$	$^1G(^2P+^2H)$	$^1G(^2P+^2G)$	$^1G(^2P+^2G)$	$^1G(^2P+^2F)$
		$^1G(^2P+^2F)$	$^3F(^2P+^4G)$	$^3F(^2P+^4F)$	$^3F(^2P+^4D)$	$^3F(^2P+^2G)$
		$^3F(^2P+^2G)$	$^3F(^2P+^2F)$	$^3F(^2P+^2F)$	$^3F(^2P+^2D)$	$^3F(^2P+^2D)$
		$^3G(^2P+^4G)$	$^3G(^2P+^4F)$	$^3G(^2P+^2H)$	$^3G(^2P+^2H)$	$^3G(^2P+^2G)$
		$^3G(^2P+^2G)$	$^3G(^2P+^2F)$	$^3G(^2P+^2F)$	$^3H(^2P+^4I)$	$^3H(^2P+^4G)$
		$^3H(^2P+^2I)$	$^3H(^2P+^2H)$	$^3H(^2P+^2H)$	$^3H(^2P+^2G)$	$^3H(^2P+^2G)$
		$^5D(^2P+^4F)$	$^5D(^2P+^4D)$	$^5F(^2P+^4G)$	$^5F(^2P+^4F)$	$^5F(^2P+^4D)$
		$^5G(^2P+^4G)$	$^5G(^2P+^4F)$	$^5H(^2P+^4I)$	$^5H(^2P+^4G)$	$^5I(^2P+^4I)$
5	34	$^1H(^2P+^2G)$	$^1H(^2P+^2G)$	$^1H(^2P+^2H)$	$^1H(^2P+^2H)$	$^1H(^2P+^2I)$
		$^3G(^2P+^2F)$	$^3G(^2P+^4F)$	$^3G(^2P+^4G)$	$^3G(^2P+^2F)$	$^3G(^2P+^2G)$
		$^3G(^2P+^2G)$	$^3G(^2P+^2H)$	$^3G(^2P+^2H)$	$^3H(^2P+^2I)$	$^3H(^2P+^2G)$
		$^3H(^2P+^2G)$	$^3H(^2P+^2H)$	$^3H(^2P+^2H)$	$^3H(^2P+^4G)$	$^3H(^2P+^4I)$
		$^3I(^2P+^2H)$	$^3I(^2P+^2H)$	$^3I(^2P+^2I)$	$^3I(^2P+^2K)$	$^3I(^2P+^4I)$
		$^5F(^2P+^4D)$	$^5F(^2P+^4G)$	$^5F(^2P+^4F)$	$^5G(^2P+^4G)$	$^5G(^2P+^4F)$
		$^5H(^2P+^4G)$	$^5H(^2P+^4I)$	$^5I(^2P+^4I)$	$^5K(^2P+^4I)$	
6	26	$^1I(^2P+^2K)$	$^1I(^2P+^2I)$	$^1I(^2P+^2H)$	$^1I(^2P+^2H)$	$^3H(^2P+^2G)$
		$^3H(^2P+^2G)$	$^3H(^2P+^2H)$	$^3H(^2P+^2H)$	$^3H(^2P+^2I)$	$^3H(^2P+^4G)$
		$^3H(^2P+^4I)$	$^3I(^2P+^4I)$	$^3I(^2P+^2K)$	$^3I(^2P+^2I)$	$^3I(^2P+^2H)$
		$^3I(^2P+^2H)$	$^3K(^2P+^2I)$	$^3K(^2P+^2K)$	$^3K(^2P+^2L)$	$^3K(^2P+^4I)$
		$^5G(^2P+^4G)$	$^5G(^2P+^4F)$	$^5H(^2P+^4G)$	$^5H(^2P+^4I)$	$^5I(^2P+^4I)$
		$^5K(^2P+^4I)$				
7	18	$^1K(^2P+^2L)$	$^1K(^2P+^2K)$	$^1K(^2P+^2I)$	$^3I(^2P+^2H)$	$^3I(^2P+^2H)$
		$^3I(^2P+^2I)$	$^3I(^2P+^2K)$	$^3I(^2P+^4I)$	$^3K(^2P+^4I)$	$^3K(^2P+^2K)$
		$^3K(^2P+^2I)$	$^3K(^2P+^2L)$	$^3L(^2P+^2L)$	$^3L(^2P+^2K)$	$^5H(^2P+^4G)$
		$^5H(^2P+^4I)$	$^5I(^2P+^4I)$	$^5K(^2P+^4I)$		
8	11	$^1L(^2P+^2K)$	$^1L(^2P+^2L)$	$^3K(^2P+^4I)$	$^3K(^2P+^2K)$	$^3K(^2P+^2I)$
		$^3K(^2P+^2L)$	$^3L(^2P+^2L)$	$^3L(^2P+^2K)$	$^3M(^2P+^2L)$	$^5I(^2P+^4I)$
		$^5K(^2P+^4I)$				
9	5	$^3L(^2P+^2L)$	$^3L(^2P+^2K)$	$^5K(^2P+^4I)$	$^3M(^2P+^2L)$	$^1M(^2P+^2L)$
10	1	$^3M(^2P+^2L)$				

Table III:- Allowed LS Term values of $4f^36s$.

Terms	-----	1P	1D	1F	1G	1H	1I	1K	1L
Quantity	-----	1	2	2	2	2	1	1	1
Terms	3S	3P	3D	3F	3G	3H	3I	3K	3L
Quantity	1	1	3	3	3	2	2	1	1
Terms	5S	-----	5D	5F	5G	-----	5I	-----	-----
Quantity	1	-----	1	1	1	-----	1	-----	-----

Table IV:- Designation of Fine levels corresponds to $4f^36s$.

J	Frequency	Terms				
0	2	$^3P(^2P+^2S)$	$^5D(^4D+^2S)$			

1	8	$^1P(^2P+^2S)$	$^3S(^4S+^2S)$	$^3P(^2P+^2S)$	$^3D(^2D+^2S)$	$^3D(^2D+^2S)$
		$^3D(^4D+^2S)$	$^5D(^4D+^2S)$	$^5F(^4F+^2S)$		
2	13	$^5S(^2S+^4S)$	$^1D(^2S+^2D)$	$^1D(^2S+^2D)$	$^3P(^2S+^2P)$	$^3D(^2D+^2S)$
		$^3D(^2D+^2S)$	$^3D(^4D+^2S)$	$^3F(^2S+^2F)$	$^3F(^2S+^2F)$	$^3F(^2S+^4F)$
		$^5D(^4D+^2S)$	$^5F(^4F+^2S)$	$^5G(^4G+^2S)$		
3	14	$^3D(^2D+^2S)$	$^3D(^2D+^2S)$	$^3D(^4D+^2S)$	$^1F(^2F+^2S)$	$^1F(^2F+^2S)$
		$^3F(^2S+^2F)$	$^3F(^2S+^2F)$	$^3F(^2S+^4F)$	$^3G(^2S+^4G)$	$^3G(^2S+^2G)$
		$^3G(^2S+^2G)$	$^5G(^2S+^4G)$	$^5D(^4D+^2S)$	$^5F(^2S+^4F)$	
4	14	$^1G(^2S+^2G)$	$^1G(^2S+^2G)$	$^3F(^2S+^2F)$	$^3F(^2S+^2F)$	$^3F(^2S+^4F)$
		$^3G(^2S+^4G)$	$^3G(^2S+^2G)$	$^3G(^2S+^2G)$	$^3H(^2S+^2H)$	$^3H(^2S+^2H)$
		$^5D(^4D+^2S)$	$^5F(^2S+^4F)$	$^5G(^2S+^4G)$	$^5I(^2S+^4I)$	
5	12	$^1H(^2S+^2H)$	$^1H(^2S+^2H)$	$^3G(^2S+^4G)$	$^3G(^2S+^2G)$	$^3G(^2S+^2G)$
		$^3H(^2S+^2H)$	$^3H(^2S+^2H)$	$^3I(^2S+^4I)$	$^3I(^2S+^2I)$	$^5F(^2S+^4F)$
		$^5G(^2S+^4G)$	$^5I(^2S+^4I)$			
6	8	$^1I(^2S+^2I)$	$^3H(^2S+^2H)$	$^3H(^2S+^2H)$	$^3I(^2S+^4I)$	$^3I(^2S+^2I)$
		$^3K(^2S+^2K)$	$^5G(^2S+^4G)$	$^5I(^2S+^4I)$		
7	6	$^1K(^2S+^2K)$	$^3I(^2S+^4I)$	$^3I(^2S+^2I)$	$^3K(^2S+^2K)$	$^3L(^2S+^2L)$
		$^5I(^2S+^4I)$				
8	4	$^1L(^2S+^2L)$	$^3K(^2S+^2K)$	$^3L(^2S+^2L)$	$^5I(^2S+^4I)$	
9	1	$^3L(^2S+^2L)$				

Table V: Term Energies of $4f^25d^2$ configuration.

$E(f2d2;1G)=-0.0051F2(nf;nd)-0.0668F4(nf;nd)$	1
$E(f2d2;3G)=-0.0051F2(nf;nd)-0.0668F4(nf;nd)$	2
$E(f2d2;5G)=-0.0051F2(nf;nd)-0.0668F4(nf;nd)$	3
$E(f2d2;3G)=0.0117F2(nf;nd)-0.0678F4(nf;nd)-0.0758G1(nf;nd)-0.0972G3(nf;nd)+0.0215G5(nf;nd)$	4
$E(f2d2;1H)=-0.013F2(nf;nd)-0.1039F4(nf;nd)$	5
$E(f2d2;1H)=-0.0151F2(nf;nd)-0.055F4(nf;nd)$	6
$E(f2d2;1F)=0.0204F2(nf;nd)-0.1224F4(nf;nd)$	7
$E(f2d2;1F)=0.0204F2(nf;nd)-0.1224F4(nf;nd)$	8
$E(f2d2;3H)=-0.0242F2(nf;nd)-0.0551F4(nf;nd)+0.0237G3(nf;nd)+0.0561G5(nf;nd)$	9
$E(f2d2;3F)=0.026F2(nf;nd)-0.0815F4(nf;nd)+0.127G1(nf;nd)+0.1275G3(nf;nd)-0.0109G5(nf;nd)$	10
$E(f2d2;3F)=0.026F2(nf;nd)-0.0815F4(nf;nd)+0.127G1(nf;nd)+0.1275G3(nf;nd)-0.0109G5(nf;nd)$	11
$E(f2d2;1M)=-0.0364F2(nf;nd)-0.0703F4(nf;nd)$	12
$E(f2d2;1G)=-0.0388F2(nf;nd)-0.0378F4(nf;nd)$	13
$E(f2d2;1F)=-0.0444F2(nf;nd)-0.0303F4(nf;nd)$	14
$E(f2d2;3F)=-0.0444F2(nf;nd)-0.0303F4(nf;nd)$	15
$E(f2d2;5F)=-0.0444F2(nf;nd)-0.0303F4(nf;nd)$	16
$E(f2d2;3L)=-0.049F2(nf;nd)-0.0678F4(nf;nd)-0.3384G1(nf;nd)+0.1036G3(nf;nd)+0.0425G5(nf;nd)$	17
$E(f2d2;1D)=0.04F2(nf;nd)$	18
$E(f2d2;3D)=0.04F2(nf;nd)$	19
$E(f2d2;5D)=0.04F2(nf;nd)$	20
$E(f2d2;1F)=0.0563F2(nf;nd)-0.0767F4(nf;nd)$	21
$E(f2d2;3F)=0.0571F2(nf;nd)+0.4667G1(nf;nd)+0.0551G3(nf;nd)$	22
$E(f2d2;3F)=0.0571F2(nf;nd)+0.4667G1(nf;nd)+0.0551G3(nf;nd)$	23
$E(f2d2;3D)=0.0571F2(nf;nd)-0.1429F4(nf;nd)-0.0429G1(nf;nd)-0.1143G3(nf;nd)+0.1299G5(nf;nd)$	24
$E(f2d2;3D)=0.0571F2(nf;nd)-0.1429F4(nf;nd)-0.0429G1(nf;nd)-0.1143G3(nf;nd)+0.1299G5(nf;nd)$	25
$E(f2d2;1D)=-0.0612F2(nf;nd)+0.0816F4(nf;nd)$	26
$E(f2d2;1K)=-0.0661F2(nf;nd)-0.0634F4(nf;nd)$	27
$E(f2d2;1G)=0.0667F2(nf;nd)$	28
$E(f2d2;1G)=0.0667F2(nf;nd)$	29
$E(f2d2;3G)=0.0667F2(nf;nd)$	30
$E(f2d2;3G)=0.0667F2(nf;nd)$	31
$E(f2d2;5G)=0.0667F2(nf;nd)$	32

$E(f2d2;5G)=0.0667F2(nf;nd)$	33
$E(f2d2;3L)=-0.0667F2(nf;nd)-0.0642F4(nf;nd)-0.0999G3(nf;nd)+0.0734G5(nf;nd)$	34
$E(f2d2;3H)=-0.0699F2(nf;nd)-0.0081F4(nf;nd)+0.1768G1(nf;nd)+0.0891G3(nf;nd)-0.0506G5(nf;nd)$	35
$E(f2d2;1G)=0.0711F2(nf;nd)-0.0687F4(nf;nd)$	36
$E(f2d2;3H)=0.0727F2(nf;nd)+0.2222G3(nf;nd)+0.028G5(nf;nd)$	37
$E(f2d2;3H)=0.0727F2(nf;nd)+0.2222G3(nf;nd)+0.028G5(nf;nd)$	38
$E(f2d2;1I)=0.0769F2(nf;nd)$	39
$E(f2d2;3I)=0.0769F2(nf;nd)$	40
$E(f2d2;5I)=0.0769F2(nf;nd)$	41
$E(f2d2;1K)=-0.0769F2(nf;nd)-0.0606F4(nf;nd)$	42
$E(f2d2;3K)=-0.0769F2(nf;nd)-0.0606F4(nf;nd)$	43
$E(f2d2;5K)=-0.0769F2(nf;nd)-0.0606F4(nf;nd)$	44
$E(f2d2;3G)=-0.0814F2(nf;nd)+0.0106F4(nf;nd)-0.127G1(nf;nd)-0.0614G3(nf;nd)+0.077G5(nf;nd)$	45
$E(f2d2;3G)=-0.0814F2(nf;nd)+0.0106F4(nf;nd)-0.127G1(nf;nd)-0.0614G3(nf;nd)+0.077G5(nf;nd)$	46
$E(f2d2;1G)=0.0816F2(nf;nd)+0.0023F4(nf;nd)$	47
$E(f2d2;1D)=0.0844F2(nf;nd)-0.0909F4(nf;nd)$	48
$E(f2d2;3D)=0.0844F2(nf;nd)-0.0909F4(nf;nd)$	49
$E(f2d2;5D)=0.0844F2(nf;nd)-0.0909F4(nf;nd)$	50
$E(f2d2;1I)=-0.0874F2(nf;nd)+0.0105F4(nf;nd)$	51
$E(f2d2;3K)=0.08F2(nf;nd)+0.1469G5(nf;nd)$	52
$E(f2d2;3I)=-0.0909F2(nf;nd)-0.0553F4(nf;nd)-0.3016G1(nf;nd)+0.1204G3(nf;nd)+0.0318G5(nf;nd)$	53
$E(f2d2;3I)=-0.0909F2(nf;nd)-0.0553F4(nf;nd)-0.3016G1(nf;nd)+0.1204G3(nf;nd)+0.0318G5(nf;nd)$	54
$E(f2d2;3G)=0.0909F2(nf;nd)-0.0698F4(nf;nd)+0.0149G3(nf;nd)-0.0101G5(nf;nd)$	55
$E(f2d2;3H)=0.0952F2(nf;nd)+0.0043F4(nf;nd)+0.4714G1(nf;nd)+0.0508G3(nf;nd)+0.0223G5(nf;nd)$	56
$E(f2d2;3H)=0.0952F2(nf;nd)+0.0043F4(nf;nd)+0.4714G1(nf;nd)+0.0508G3(nf;nd)+0.0223G5(nf;nd)$	57
$E(f2d2;1H)=-0.0991F2(nf;nd)+0.0303F4(nf;nd)$	58
$E(f2d2;3H)=-0.0991F2(nf;nd)+0.0303F4(nf;nd)$	59
$E(f2d2;5H)=-0.0991F2(nf;nd)+0.0303F4(nf;nd)$	60
$E(f2d2;3F)=0.1009F2(nf;nd)-0.0586F4(nf;nd)+0.0859G1(nf;nd)+0.1064G3(nf;nd)+0.0624G5(nf;nd)$	61
$E(f2d2;1I)=0.1039F2(nf;nd)+0.006F4(nf;nd)$	62
$E(f2d2;1I)=0.1039F2(nf;nd)+0.006F4(nf;nd)$	63
$E(f2d2;3F)=-0.1048F2(nf;nd)+0.0952F4(nf;nd)+0.2143G1(nf;nd)+0.0794G3(nf;nd)+0.0577G5(nf;nd)$	64
$E(f2d2;3F)=-0.1048F2(nf;nd)+0.0952F4(nf;nd)+0.2143G1(nf;nd)+0.0794G3(nf;nd)+0.0577G5(nf;nd)$	65
$E(f2d2;3I)=-0.1091F2(nf;nd)+0.0413F4(nf;nd)-0.0045G3(nf;nd)-0.0645G5(nf;nd)$	66
$E(f2d2;3K)=0.1099F2(nf;nd)+0.0073F4(nf;nd)+0.2381G3(nf;nd)+0.0206G5(nf;nd)$	67
$E(f2d2;1I)=0.1111F2(nf;nd)+0.0083F4(nf;nd)$	68
$E(f2d2;3I)=0.1111F2(nf;nd)+0.0083F4(nf;nd)$	69
$E(f2d2;5I)=0.1111F2(nf;nd)+0.0083F4(nf;nd)$	70
$E(f2d2;1H)=-0.1111F2(nf;nd)-0.0468F4(nf;nd)$	71
$E(f2d2;3H)=-0.1111F2(nf;nd)-0.0468F4(nf;nd)$	72
$E(f2d2;5H)=-0.1111F2(nf;nd)-0.0468F4(nf;nd)$	73
$E(f2d2;1F)=0.1111F2(nf;nd)-0.0606F4(nf;nd)$	74
$E(f2d2;3F)=0.1111F2(nf;nd)-0.0606F4(nf;nd)$	75
$E(f2d2;5F)=0.1111F2(nf;nd)-0.0606F4(nf;nd)$	76
$E(f2d2;3G)=-0.1111F4(nf;nd)+0.0144G3(nf;nd)-0.0505G5(nf;nd)$	77
$E(f2d2;1H)=-0.1122F2(nf;nd)+0.047F4(nf;nd)$	78
$E(f2d2;1L)=0.1143F2(nf;nd)+0.0084F4(nf;nd)$	79
$E(f2d2;1K)=-0.1143F2(nf;nd)-0.0476F4(nf;nd)$	80
$E(f2d2;1L)=-0.1192F2(nf;nd)+0.0313F4(nf;nd)$	81
$E(f2d2;1G)=-0.1206F2(nf;nd)+0.1002F4(nf;nd)$	82
$E(f2d2;1G)=-0.1206F2(nf;nd)+0.1002F4(nf;nd)$	83
$E(f2d2;3I)=-0.1209F2(nf;nd)-0.044F4(nf;nd)-0.0649G3(nf;nd)+0.0646G5(nf;nd)$	84
$E(f2d2;3K)=0.1212F2(nf;nd)+0.0114F4(nf;nd)+0.4762G1(nf;nd)+0.0626G3(nf;nd)+0.0129G5(nf;nd)$	85
$E(f2d2;3K)=0.1212F2(nf;nd)+0.0114F4(nf;nd)+0.4762G1(nf;nd)+0.0626G3(nf;nd)+0.0129G5(nf;nd)$	86

$E(f2d2;3I)=-0.1239F2(nf;nd)+0.059F4(nf;nd)-0.1869G1(nf;nd)-0.0017G3(nf;nd)+0.0156G5(nf;nd)$	87
$E(f2d2;3K)=-0.1262F2(nf;nd)+0.0429F4(nf;nd)+0.3081G1(nf;nd)-0.0587G3(nf;nd)+0.0683G5(nf;nd)$	88
$E(f2d2;3H)=0.1273F2(nf;nd)+0.0229G5(nf;nd)$	89
$E(f2d2;1L)=0.1282F2(nf;nd)+0.014F4(nf;nd)$	90
$E(f2d2;3L)=0.1282F2(nf;nd)+0.014F4(nf;nd)$	91
$E(f2d2;5L)=0.1282F2(nf;nd)+0.014F4(nf;nd)$	92
$E(f2d2;3H)=-0.1282F2(nf;nd)+0.1026F4(nf;nd)+0.0505G3(nf;nd)+0.0944G5(nf;nd)$	93
$E(f2d2;1K)=-0.1287F2(nf;nd)+0.0629F4(nf;nd)$	94
$E(f2d2;1H)=-0.1299F2(nf;nd)-0.039F4(nf;nd)$	95
$E(f2d2;1H)=-0.1299F2(nf;nd)-0.039F4(nf;nd)$	96
$E(f2d2;1L)=0.1322F2(nf;nd)+0.0158F4(nf;nd)$	97
$E(f2d2;1I)=-0.1325F2(nf;nd)+0.1039F4(nf;nd)$	98
$E(f2d2;1G)=0.1333F2(nf;nd)$	99
$E(f2d2;3G)=0.1333F2(nf;nd)$	100
$E(f2d2;5G)=0.1333F2(nf;nd)$	101
$E(f2d2;3M)=0.1333F2(nf;nd)+0.016F4(nf;nd)+0.2498G3(nf;nd)+0.0245G5(nf;nd)$	102
$E(f2d2;1G)=-0.1333F2(nf;nd)+0.0891F4(nf;nd)$	103
$E(f2d2;3G)=-0.1333F2(nf;nd)+0.0891F4(nf;nd)$	104
$E(f2d2;5G)=-0.1333F2(nf;nd)+0.0891F4(nf;nd)$	105
$E(f2d2;1I)=-0.1334F2(nf;nd)+0.0583F4(nf;nd)$	106
$E(f2d2;3K)=-0.1345F2(nf;nd)+0.0629F4(nf;nd)+0.0696G3(nf;nd)+0.0497G5(nf;nd)$	107
$E(f2d2;3H)=0.1364G5(nf;nd)$	108
$E(f2d2;1I)=-0.1368F2(nf;nd)+0.0699F4(nf;nd)$	109
$E(f2d2;3I)=-0.1368F2(nf;nd)+0.0699F4(nf;nd)$	110
$E(f2d2;5I)=-0.1368F2(nf;nd)+0.0699F4(nf;nd)$	111
$E(f2d2;3H)=-0.1377F2(nf;nd)+0.0787F4(nf;nd)+0.2698G1(nf;nd)-0.0142G3(nf;nd)+0.0713G5(nf;nd)$	112
$E(f2d2;3H)=-0.1377F2(nf;nd)+0.0787F4(nf;nd)+0.2698G1(nf;nd)-0.0142G3(nf;nd)+0.0713G5(nf;nd)$	113
$E(f2d2;3M)=0.1399F2(nf;nd)+0.0194F4(nf;nd)+0.4798G1(nf;nd)+0.0745G3(nf;nd)+0.0134G5(nf;nd)$	114
$E(f2d2;3F)=0.1429F2(nf;nd)+0.0385G3(nf;nd)+0.1768G5(nf;nd)$	115
$E(f2d2;3F)=0.1429F2(nf;nd)+0.0385G3(nf;nd)+0.1768G5(nf;nd)$	116
$E(f2d2;3G)=-0.1429F2(nf;nd)-0.0317F4(nf;nd)-0.2429G1(nf;nd)+0.1302G3(nf;nd)+0.0289G5(nf;nd)$	117
$E(f2d2;3G)=-0.1429F2(nf;nd)-0.0317F4(nf;nd)-0.2429G1(nf;nd)+0.1302G3(nf;nd)+0.0289G5(nf;nd)$	118
$E(f2d2;3D)=0.1429F2(nf;nd)-0.039F4(nf;nd)-0.0159G1(nf;nd)-0.0779G3(nf;nd)-0.0749G5(nf;nd)$	119
$E(f2d2;3D)=0.1429F2(nf;nd)-0.039F4(nf;nd)-0.0159G1(nf;nd)-0.0779G3(nf;nd)-0.0749G5(nf;nd)$	120
$E(f2d2;1P)=0.1429F2(nf;nd)-0.1905F4(nf;nd)$	121
$E(f2d2;1N)=0.1455F2(nf;nd)+0.0222F4(nf;nd)$	122
$E(f2d2;1D)=0.1489F2(nf;nd)-0.0242F4(nf;nd)$	123
$E(f2d2;1F)=0.157F2(nf;nd)-0.0076F4(nf;nd)$	124
$E(f2d2;1F)=-0.1633F2(nf;nd)-0.0204F4(nf;nd)$	125
$E(f2d2;1D)=0.16F2(nf;nd)$	126
$E(f2d2;1D)=0.16F2(nf;nd)$	127
$E(f2d2;3D)=0.16F2(nf;nd)$	128
$E(f2d2;3D)=0.16F2(nf;nd)$	129
$E(f2d2;5D)=0.16F2(nf;nd)$	130
$E(f2d2;5D)=0.16F2(nf;nd)$	131
$E(f2d2;3D)=0.1818F2(nf;nd)+0.021F4(nf;nd)-0.0051G1(nf;nd)-0.0519G3(nf;nd)-0.0699G5(nf;nd)$	132
$E(f2d2;1G)=0.1818F2(nf;nd)+0.0404F4(nf;nd)$	133
$E(f2d2;3F)=0.1905F2(nf;nd)+0.0476F4(nf;nd)+0.0227G3(nf;nd)+0.0272G5(nf;nd)$	134
$E(f2d2;1D)=0.2041F2(nf;nd)+0.0612F4(nf;nd)$	135
$E(f2d2;1D)=0.2041F2(nf;nd)+0.0612F4(nf;nd)$	136
$E(f2d2;3F)=0.2121F2(nf;nd)+0.0771F4(nf;nd)+0.0169G3(nf;nd)+0.0116G5(nf;nd)$	137
$E(f2d2;3F)=0.2143G3(nf;nd)$	138
$E(f2d2;3F)=0.2143G3(nf;nd)$	139
$E(f2d2;1P)=0.2208F2(nf;nd)+0.0809F4(nf;nd)$	140

$E(f2d2;1D)=0.2222F2(nf;nd)+0.0909F4(nf;nd)$	141
$E(f2d2;3D)=0.2222F2(nf;nd)+0.0909F4(nf;nd)$	142
$E(f2d2;5D)=0.2222F2(nf;nd)+0.0909F4(nf;nd)$	143
$E(f2d2;3P)=0.2286F2(nf;nd)+0.0952F4(nf;nd)+0.0714G1(nf;nd)+0.0952G3(nf;nd)+0.2381G5(nf;nd)$	144
$E(f2d2;3P)=0.2286F2(nf;nd)+0.0952F4(nf;nd)+0.0714G1(nf;nd)+0.0952G3(nf;nd)+0.2381G5(nf;nd)$	145
$E(f2d2;1D)=0.2314F2(nf;nd)+0.1068F4(nf;nd)$	146
$E(f2d2;3P)=0.2381F2(nf;nd)+0.1169F4(nf;nd)+0.0476G1(nf;nd)+0.0519G3(nf;nd)+0.0849G5(nf;nd)$	147
$E(f2d2;3P)=0.2381F2(nf;nd)+0.1169F4(nf;nd)+0.0476G1(nf;nd)+0.0519G3(nf;nd)+0.0849G5(nf;nd)$	148
$E(f2d2;3P)=0.2424F2(nf;nd)+0.1259F4(nf;nd)+0.0354G1(nf;nd)+0.034G3(nf;nd)+0.049G5(nf;nd)$	149
$E(f2d2;1S)=0.2597F2(nf;nd)+0.1618F4(nf;nd)$	150
$E(f2d2;1S)=0.2667F2(nf;nd)+0.1818F4(nf;nd)$	151
$E(f2d2;3S)=0.2667F2(nf;nd)+0.1818F4(nf;nd)$	152
$E(f2d2;5S)=0.2667F2(nf;nd)+0.1818F4(nf;nd)$	153
$E(f2d2;1S)=0.2857F2(nf;nd)+0.2857F4(nf;nd)$	154
$E(f2d2;1F)=-0.2F2(nf;nd)$	155
$E(f2d2;1F)=-0.2F2(nf;nd)$	156
$E(f2d2;1H)=-0.2F2(nf;nd)$	157
$E(f2d2;3F)=-0.2F2(nf;nd)$	158
$E(f2d2;3F)=-0.2F2(nf;nd)$	159
$E(f2d2;3H)=-0.2F2(nf;nd)$	160
$E(f2d2;3I)=-0.2F2(nf;nd)$	161
$E(f2d2;5F)=-0.2F2(nf;nd)$	162
$E(f2d2;5F)=-0.2F2(nf;nd)$	163
$E(f2d2;5H)=-0.2F2(nf;nd)$	164
$E(f2d2;3P)=-0.2F2(nf;nd)+0.1333G1(nf;nd)+0.3G3(nf;nd)$	165
$E(f2d2;3P)=-0.2F2(nf;nd)+0.1333G1(nf;nd)+0.3G3(nf;nd)$	166
$E(f2d2;3G)=-0.2F2(nf;nd)-0.0159G3(nf;nd)+0.0556G5(nf;nd)$	167
$E(f2d2;3G)=-0.2F2(nf;nd)-0.0159G3(nf;nd)+0.0556G5(nf;nd)$	168
$E(f2d2;3D)=-0.2F2(nf;nd)-0.1333G1(nf;nd)+0.1286G3(nf;nd)$	169
$E(f2d2;3D)=-0.2F2(nf;nd)-0.1333G1(nf;nd)+0.1286G3(nf;nd)$	170
$E(f2d2;1P)=-0.2F2(nf;nd)+0.0303F4(nf;nd)$	171
$E(f2d2;3P)=-0.2F2(nf;nd)+0.0303F4(nf;nd)$	172
$E(f2d2;5P)=-0.2F2(nf;nd)+0.0303F4(nf;nd)$	173
$E(f2d2;1P)=-0.2F2(nf;nd)$	174
$E(f2d2;3P)=-0.2F2(nf;nd)$	175
$E(f2d2;5P)=-0.2F2(nf;nd)$	176
$E(f2d2;1S)=0.4F2(nf;nd)$	177
$E(f2d2;3S)=0.4F2(nf;nd)$	178
$E(f2d2;5S)=0.4F2(nf;nd)$	179
$E(f2d2;3P)=0.5G1(nf;nd)$	180
$E(f2d2;3P)=0.5G1(nf;nd)$	181

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