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Optical Spectra and Zeeman Effect for Pr^{3+} and Nd^{3+} in
 LuPO_4 and YPO_4

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ABSTRACT

Absorption spectra of Pr^{3+} and Nd^{3+} diluted in LuPO_4 and YPO_4 crystals have been measured from 4,000 to 30000 cm^{-1} , at liquid He and N_2 temperatures. Fluorescence was observed for Pr^{3+} and Nd^{3+} in YPO_4 , and Zeeman spectra were obtained in the visible region. The transitions were assigned and fit to a semi-empirical Hamiltonian with adjustable parameters via a least squares procedure. Satisfactory fits and reasonable agreement between calculated and measured g values were obtained.

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I. Introduction

The present study of the optical spectra of Nd^{3+} and Pr^{3+} in YPO_4 and LuPO_4 is a continuation of the characterization of possible sites where actinide (and other) impurity ions can be incorporated into these materials. Recently it has been suggested^{1,2} that synthetic analogs of the mineral monazite $[(\text{La}, \text{Ce}, \text{Nd}, \text{Y}, \dots)\text{PO}_4]$ represent possible host materials for the storage of long lived actinide ions. This potentially important application provides the motivation for studies of the chemical and physical properties of the lanthanide orthophosphate-impurity systems.

Previous work in this area includes electron paramagnetic resonance measurements (EPR) of Gd^{3+} in both the monoclinic (LaPO_4 to GdPO_4) and tetragonal zircon (TbPO_4 to LuPO_4 , YPO_4) structures.³⁻⁵ Additional EPR investigations^{6,7} have been carried out for Ce^{3+} , Nd^{3+} , Dy^{3+} , Er^{3+} , and Yb^{3+} in LuPO_4 and YPO_4 . These lanthanide ions are either direct analogs of or have properties that are directly related to the actinide ions of interest. The present work is complementary to the EPR measurements and is similar to the previously reported study of optical spectra and Zeeman effect of Er^{3+} in LuPO_4 .⁸

In the work reported here, the optical spectra of Pr^{3+} and Nd^{3+} in YPO_4 and LuPO_4 were used to deduce a set of energy levels and g values in those cases where splittings due to a magnetic field could be observed. The energy levels were assigned to states derived from the free ion f^n configuration ($n=2$ for Pr^{3+} , $n=3$ for Nd^{3+}), restricted to D_{2d} point symmetry and were fit to a semi-empirical Hamiltonian by least squares minimization. The adjustable parameters describe the

electrostatic, spin-orbit, and crystal field interactions. The assigned energy levels presented here are the best choice in terms of agreement with the calculated energies and g values, and in terms of consistency with respect to the values of the crystal field parameters among the four crystals.

II. Experimental Procedure

The Pr- and Nd-doped LuPO_4 and YPO_4 crystals employed in this work were grown by a technique^{4,5} similar to that initially described by Feigelson.⁹ In this procedure the lanthanide oxide (i.e., Lu_2O_3 or Y_2O_3 plus the Pr_2O_3 or Nd_2O_3 dopant) is mixed with PbHPO_4 and reacted at high temperature (1360°C) in a platinum crucible. Accompanying decomposition of the PbHPO_4 results in the formation of $\text{Pb}_2\text{P}_2\text{O}_7$, which then serves as a flux during the subsequent crystal growth via spontaneous nucleation during slow cooling (1°C/h).

The absorption spectra of the crystals between 11,000 and 30,000 cm^{-1} were photographed on a 3.4m Ebert spectrograph with a dispersion of about $5.2 \text{ \AA/mm}$, and the transitions between 4,000 and 11,000 cm^{-1} were scanned on a Cary model 17 spectrophotometer. These observations were made at approximately 2.0 K and at 77 K. The photographic measurements were repeated with the crystal in a magnetic field of 25.9 kG, with the c axis parallel and perpendicular to the field. Fluorescence spectra were excited with a pulsed dye laser and then recorded photographically on a fast (f/6) .75m spectrograph, and photoelectrically on a .85m scanning monochromator with both dc and photon counting detection modes. All spectra were analyzed with a linear polarizer oriented in both the parallel and perpendicular directions relative to the c axis of the

crystal.

The spectra are well characterized by their group theoretical selection rules, and the D_{2d} symmetry sites of the YPO_4 and $LuPO_4$ hosts are so similar that the wavelengths and relative intensities of the lines of Pr^{3+} (or Nd^{3+}) are nearly identical in each crystal. Because of this, features of the spectra specific to Pr^{3+} and Nd^{3+} can be discussed with respect to both hosts at the same time.

A. Pr^{3+}

For an even number of electrons such as Pr^{3+} (f^2), the crystal field eigenstates carry the Γ_1 through Γ_5 point group representations associated with the D_{2d} site symmetry. Selection rules for the allowed electric dipole transitions reduce to:

$$\left. \begin{array}{l} \Gamma_1(\Gamma_2) \leftrightarrow \Gamma_4(\Gamma_3) \\ \Gamma_5 \leftrightarrow \Gamma_5 \end{array} \right\} \quad (\text{pol.} \parallel \text{c axis})$$

$$\Gamma_5 \leftrightarrow \Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4 \quad (\text{pol.} \perp \text{c axis})$$

At about 2.0 K for both host materials, the strong transition in the parallel polarization from the ground state to the $(^3P_0)\Gamma_1$ at $\sim 20450 \text{ cm}^{-1}$ clearly identifies the ground state as $(^3H_4)\Gamma_4$. At 77 K, transitions from a low lying Γ_5 (139 cm^{-1} in YPO_4 ; 143 cm^{-1} in $LuPO_4$) are readily apparent. Because the $Pr^{3+}:LuPO_4$ crystals are smaller (typically $2\text{mm} \times 10\text{mm} \times .5\text{mm}$, about half the size of a typical $Pr^{3+}:YPO_4$ crystal) and their absorption spectra are considerably weaker, only the $Pr^{3+}:YPO_4$ crystals were studied in great detail.

The $\text{Pr}^{3+}:\text{YPO}_4$ crystal studied had a rich spectrum in the near infrared at liquid N_2 temperature. The transitions between the ${}^3\text{H}_4$ and the ${}^3\text{F}_{2,3,4}$ multiplets provide evidence for a Γ_1 level at 100 cm^{-1} and a Γ_2 level at 150 cm^{-1} , although further confirmation would be desirable. Additional spectra involving the ${}^3\text{H}_{5,6}$ and the ${}^3\text{F}_{2,3,4}$ crystal field levels were obtained by observing fluorescence associated with pumping the $({}^1\text{D}_2)\Gamma_5$, $({}^3\text{P}_0)\Gamma_1$, and the $({}^3\text{P}_1)\Gamma_{1,5}$ field levels with a tunable pulsed dye laser. The majority of the fluorescent transitions originate from the $({}^3\text{P}_0)\Gamma_1$ level, although the signature of fluorescence is always a strong transition with an energy of 16315.9 cm^{-1} . At present, we are unable to classify this transition, which appears when the $({}^1\text{D}_2)\Gamma_5$ level is pumped and shows no Zeeman splitting. This indicates perhaps, that it originates from the $({}^1\text{D}_2)\Gamma_3$ level. The 16315.9 cm^{-1} energy, however, does not correspond closely with any difference between levels predicted by our calculations. The experimentally determined energy levels and g values are displayed in Table I.

B. Nd^{3+}

For an odd number of electrons, as in the case of $\text{Nd}^{3+} (4f^3)$, the crystal field eigenstates carry the Γ_6 and Γ_7 double group representations associated with the D_{2d} site symmetry. Selection rules for point group symmetry allowed electric dipole transitions reduce to:

$$\Gamma_7 \leftrightarrow \Gamma_6 \quad (\text{pol.} \parallel \text{c axis})$$

$$\Gamma_6, \Gamma_7 \leftrightarrow \Gamma_6, \Gamma_7 \quad (\text{pol.} \perp \text{c axis})$$

For both of the host crystals, the transitions used to assign energy levels clearly obeyed these selection rules. With polarization

parallel to the c axis of the crystals, a number of weaker satellite transitions appeared around the ${}^4F_{3/2}$ ($\sim 11,400 \text{ cm}^{-1}$) and ${}^4F_{5/2}$ ($\sim 12,400 \text{ cm}^{-1}$) transitions. The satellites near the strong transitions corresponding to the pair of ${}^4F_{3/2}$ crystal field levels are within 10 cm^{-1} , so they are likely to be vibronic in nature. In addition, the $\text{Nd}^{3+}:\text{YPO}_4$ crystal has weak absorption lines at 16003 cm^{-1} and 17351 cm^{-1} that do not fit into our analysis. By pumping the $({}^4G_{7/2})\Gamma_6$ level of $\text{Nd}^{3+}:\text{LuPO}_4$ at 18885.3 cm^{-1} with a pulsed dye laser, we were able to observe fluorescence from the ${}^4F_{3/2}$ pair of crystal field levels to the ground state and the first excited (120 cm^{-1}) states. Some very broad fluorescence features were also seen at about 240 cm^{-1} , but individual lines could not be identified. Experimentally determined energy levels and g values are displayed in Table II.

III. Analysis and Discussion

The electronic states resulting from an f^n configuration restricted to D_{2d} Symmetry can be described with an effective Hamiltonian of the form¹⁰:

$$H = H_1 + H_2 + H_3 + H_4 \quad (1)$$

where

$$H_1 = F^0 + \sum_{k=2,4,6} F^k(4f,4f) \sum_{i>j=1}^n C^k(i) \cdot C^k(j) \quad (2)$$

$$H_2 = \sum_{i=1}^n \xi_{4f} \vec{L}_i \cdot \vec{s}_i \quad (3)$$

$$H_3 = \sum_{i=1}^n B_0^2 C_0^2(i) + B_0^4 C_0^4(i) + B_4^4 \left[C_4^4(i) + C_{-4}^4(i) \right] \\ B_0^6 C_0^6(i) + B_4^6 \left[C_4^6(i) + C_{-4}^6(i) \right] \quad (4)$$

$$H_4 = \alpha \vec{L}^2 + \beta G(G_2) + \gamma G(R_7) + \dots \quad (5)$$

where $G(G_2)$ and $G(R_7)$ are representations of Casimir's operator for the groups G_2 and R_7 on the appropriate manifold. In addition H_4 contains terms parameterizing three body interactions (T^k), and magnetic terms (M^k, P^k).^{10,11}

The thirteen parameters explicitly contained in equations (2-5) were adjusted to give the best fit to the experimental energy levels in each case using the least squares criterion. Because of the limited data obtained for $\text{Pr}^{3+}:\text{LuPO}_4$, however, the α , β , and γ parameters were not varied, but held fixed at the values obtained for $\text{Pr}^{3+}:\text{YPO}_4$. The additional parameters contained in H_4 were also fixed at the values obtained for each ion in LaCl_3 .¹¹ Results of the calculations are compared with the experimentally determined quantities for Pr^{3+} in Table I and for Nd^{3+} in Table II.

To identify the crystal field levels, the two basis vectors with the largest percentage composition are given in Table I and Table II. For Nd^{3+} , the basis vectors are denoted $(2S+1)LQ(2J, 2J_z)$, where Q is an additional quantum number used to distinguish multiply occurring SL multiplets.¹² Each crystal field level is a Kramers doublet, with the Γ_7 representation carried by basis vectors with $(J_z)_{\text{mod } 4} = \pm 1/2$, and the Γ_6 representation carried by basis vectors with $(J_z)_{\text{mod } 4} = \pm 3/2$. The Pr^{3+} basis vectors are denoted $(2S+1)L(J, [J_z])$ (the Q quantum number is

not needed), where the change from $SLJ J_z$ coupling has been made:

$$|J, [J_z]\rangle = \begin{cases} |J, J_z\rangle; J_z=0, \text{ or } J_z \text{ odd} \\ \frac{1}{\sqrt{2}} \left[|J, J_z\rangle + \frac{[J_z]}{|J_z|} |J, J_z\rangle \right]; J_z=2, 4, \dots \end{cases}$$

where $[J_z] = \pm |J_z|$. Each of these transformed states has definite time reversal symmetry and carries an irreducible representation of D_{2d} , except for the odd values of J_z , where an $(SL)J, \pm |J_z|$ pair of states carries a doubly degenerate Γ_5 representation.

Agreement between the experimental energies and g values and the corresponding quantities calculated from the semi-empirical model was satisfactory in most cases. There were, however, some obvious discrepancies. In particular for $Pr^{3+}:YPO_4$, the level assigned to $(^3F_2)\Gamma_4$ (5015.7 cm^{-1}) seems to have an abnormally large deviation from the calculated value, but evidence for this level comes from both absorption and fluorescence spectra. The corresponding absorption line from the lowest lying $(^3H_4)\Gamma_5$ level is also seen in $Pr^{3+}:LuPO_4$, with a correspondingly large deviation from the calculated value. Another surprising discrepancy is represented by the small observed g value of the $(^1D_2)\Gamma_5$ level of the $Pr^{3+}:YPO_4$ crystal. Nearly all of the observed g values for all four crystals are consistent with rather pure $(SL)J$ composition of the crystal field levels, making this splitting anomalously small and difficult to explain.

Except for the previously described features of the Nd^{3+} spectrum, the model fits well with the experimental observations for both host

materials. Many of the lines of $\text{Nd}^{3+}:\text{YPO}_4$ and $\text{Nd}^{3+}:\text{LuPO}_4$ are displaced when the magnetic field was applied perpendicular to the c axis, such that mixing with nearby crystal field levels is indicated. Thus, some of the pairs of lines measured in the perpendicular magnetic field that appear to have the same centers of gravity as their corresponding zero field lines may also be perturbed. This might account for the fact that the agreement between the observed and calculated perpendicular g values is slightly poorer than for the parallel g values. EPR measurements of the Nd^{3+} ground state g values yielded the following results: $g_{\parallel} = 2.842(2)$, $g_{\perp} = 1.339(1)$ for LuPO_4 and $g_{\parallel} = 3.092(2)$, $g_{\perp} = 1.224(1)$ for YPO_4 . For Nd^{3+} in LuPO_4 and YPO_4 , the agreement between the calculated and experimental g values obtained from EPR measurements in both the parallel and perpendicular field configurations is very satisfying.

The experimentally derived parameters and the reduced rms energy deviations for each fit are given in Table III, along with the previously reported parameters for Er^{3+} . The consistency among the empirical crystal field parameters for all three ions presented in Table III is satisfying, especially when considered along with their statistical errors derived from the fits. The B_0^2 parameter is perhaps most sensitive to the particular lanthanide ion, although both B_0^2 and B_0^4 appear to be sensitive to the differences between the YPO_4 and LuPO_4 . The B_4^6 parameter is probably not well determined for any of the crystals, but is especially ill-defined for Pr^{3+} , because the experimental data are comprised mainly of crystal field levels constructed from free ion states with small J values.

Work is currently in progress on Ho^{3+} , Yb^{3+} , and Tm^{3+} in these same host materials to provide parameters from additional members of the lanthanide series and to establish trends for all the crystal field parameters. With the analysis of a number of lanthanide ions in YPO_4 and LuPO_4 , the analysis of the spectra of the corresponding actinide ions should be easier. Crystals of $\text{U}^{3+}:\text{LuPO}_4$ are already available and preliminary investigations are in progress.

IV. Acknowledgements

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Table I

Pr ³⁺ :YPO ₄										Pr ³⁺ :LuPO ₄											
Sym	Energy (cm ⁻¹)		Splitting Factors				Eigenvector Composition				Sym	Energy (cm ⁻¹)		Splitting Factors				Eigenvector Composition			
			g		g _⊥		SLQ(J, [J _z])		SLQ(J, [J _z])					g		g _⊥		SLQ(J, [J _z])		SLQ(J, [J _z])	
	cal	obs	cal	obs	cal	obs	%	largest	%	second		cal	obs	cal	obs	cal	obs	%	largest	%	second
Γ ₄	0	0	0.		0.		97	3H (4, -2)	2	1G (4, -2)	Γ ₄	0	0	0.		0.		97	3H (4, -2)	2	1G (4, -2)
Γ ₁	102	100	0.		0.		81	3H (4, 4)	15	3H (4, 0)	Γ ₁	97		0.		0.		75	3H (4, 4)	21	3H (4, 0)
Γ ₅	137	139	.15		0.		73	3H (4, -1)	22	3H (4, 3)	Γ ₅	142	143	-2.1		0.		78	3H (4, -1)	17	3H (4, 3)
Γ ₂	147	150	0.		0.		84	3H (4, -4)	5	3P (1, 0)	Γ ₂	166		0.		0.		71	3H (4, -4)	12	3H (6, -4)
Γ ₃	239		0.		0.		97	3H (4, 2)	2	1G (4, 2)	Γ ₃	181		0.		0.		97	3H (4, 2)	2	1G (4, 2)
Γ ₁	349		0.		0.		80	3H (4, 0)	15	3H (4, 4)	Γ ₅	387		3.94		0.		77	3H (4, 3)	17	3H (4, -1)
Γ ₅	392		3.51		0.		73	3H (4, 3)	22	3H (4, -1)	Γ ₁	397		0.		0.		74	3H (4, 0)	21	3H (4, 4)
Γ ₃	2191		0.		0.		99	3H (5, -2)			Γ ₃	2199		0.		0.		99	3H (5, -2)		
Γ ₅	2207	2209	-3.46		0.		40	3H (5, -5)	34	3H (5, -1)	Γ ₅	2223		-3.05		0.		40	3H (5, -1)	35	3H (5, -5)
Γ ₅	2255		-4.42		0.		56	3H (5, -5)	28	3H (5, 3)	Γ ₅	2300		-3.62		0.		55	3H (5, -5)	37	3H (5, 3)
Γ ₂	2295		0.		0.		56	3H (5, 0)	40	3H (5, 4)	Γ ₂	2328		0.		0.		54	3H (5, 0)	41	3H (5, 4)
Γ ₄	2353		0.		0.		98	3H (5, 2)			Γ ₄	2338		0.		0.		98	3H (5, 2)		
Γ ₅	2409		1.58		0.		49	3H (5, -1)	46	3H (5, 3)	Γ ₅	2419		.32		0.		51	3H (5, -1)	37	3H (5, 3)
Γ ₁	2409		0.		0.		98	3H (5, -4)			Γ ₁	2436		0.		0.		97	3H (5, -4)		
Γ ₂	2499		0.		0.		42	3H (5, 0)	56	3H (5, 4)	Γ ₂	2540		0.		0.		41	3H (5, 0)	56	3H (5, 4)
Γ ₄	4269	4272	0.		0.		79	3H (6, -2)	17	3H (6, -6)	Γ ₄	4266		0.		0.		71	3H (6, -2)	22	3H (6, -6)
Γ ₅	4307	4309	5.11	4.56	0.		80	3H (6, 3)	17	3H (6, -1)	Γ ₅	4313	4306	5.90		0.		87	3H (6, 3)	9	3H (6, -1)
Γ ₃	4350		0.		0.		95	3H (6, 6)	3	3H (6, 2)	Γ ₃	4366		0.		0.		71	3H (6, 6)	26	3H (6, 2)
Γ ₄	4372	4363	0.		0.		81	3H (6, -6)	15	3H (6, -2)	Γ ₄	4453		0.		0.		76	3H (6, -6)	19	3H (6, -2)
Γ ₁	4422		0.		0.		33	3H (6, 0)	63	3H (6, 4)	Γ ₁	4453		0.		0.		66	3H (6, 4)	30	3H (6, 0)
Γ ₃	4519		0.		0.		88	3H (6, 2)	6	3F (2, 2)	Γ ₃	4530		0.		0.		65	3H (6, 2)	27	3H (6, 6)
Γ ₂	4528		0.		0.		66	3P (1, 0)	22	1I (6, -4)	Γ ₂	4555		0.		0.		32	3P (1, 0)	51	1I (6, -4)
Γ ₅	4585		-1.89		0.		69	3H (6, -1)	17	3H (6, 3)	Γ ₅	4594		-2.67		0.		76	3H (6, -1)	11	3H (6, -5)
Γ ₁	4670		0.		0.		56	3H (6, 0)	34	3H (6, 4)	Γ ₁	4699		0.		0.		55	3H (6, 0)	31	3H (6, 4)
Γ ₅	4738		-10.43		0.		85	3H (6, -5)	11	3H (6, -1)	Γ ₅	4818		-10.18		0.		82	3H (6, -5)	11	3H (6, -1)
Γ ₄	5053	5016	0.		0.		93	3F (2, -2)	3	3H (6, -2)	Γ ₄	5080	5029	0.		0.		89	3F (2, -2)	7	3H (6, -2)
Γ ₅	5069	5076	-1.44		0.		95	3F (2, -1)	2	1D (2, -1)	Γ ₅	5091	5101	-1.70		0.		91	3F (2, -1)	3	3H (6, -5)
Γ ₁	5082	5097	0.		0.		87	3F (2, 0)	8	3H (6, 0)	Γ ₁	5117	5125	0.		0.		81	3F (2, 0)	12	3H (6, 0)
Γ ₃	5110	5111	0.		0.		90	3F (2, 2)	6	3H (6, 2)	Γ ₃	5118		0.		0.		90	3F (2, 2)	6	3H (6, 2)
Γ ₂	6342	6349	0.		0.		92	3F (3, 0)	2	3P (1, 0)	Γ ₂	6345		0.		0.		97	3F (3, 0)	0	3F (4, -4)
Γ ₃	6395	6388	0.		0.		97	3F (3, -2)			Γ ₃	6394		0.		0.		96	3F (3, -2)		
Γ ₄	6446	6461	0.		0.		98	3F (3, 2)			Γ ₅	6465	6450	5.93		0.		91	3F (3, 3)	3	3F (3, -1)

Γ_5	6448	6442	6.28	0.	97 3F (3, 3) 0 3H (6, 3)	Γ_4	6469	6458	0.	0.	99 3F (3, 2)
Γ_5	6521	6503	-1.78	0.	95 3F (3, -1) 1 3H (6, -1)	Γ_5	6569	6527	-1.28	0.	88 3F (3, -1) 4 3F (3, 3)
Γ_1	6775	6779	0.	0.	32 3F (4, 0) 21 1G (4, 0)	Γ_1	6771	6792	0.	0.	32 3F (4, 0) 23 1G (4, 0)
Γ_5	6821	6829	2.26	0.	29 3F (4, 3) 28 3F (4, -1)	Γ_5	6799		2.86	0.	31 3F (4, 3) 22 1G (4, 3)
Γ_4	6861	6862	0.	0.	67 3F (4, -2) 30 1G (4, -2)	Γ_4	6842		0.	0.	65 3F (4, -2) 32 1G (4, -2)
Γ_2	6875	6886	0.	0.	64 3F (4, -4) 32 1G (4, -4)	Γ_2	6855		0.	0.	62 3F (4, -4) 33 1G (4, -4)
Γ_1	6933	6940	0.	0.	26 3F (4, 0) 37 3F (4, 4)	Γ_1	6892		0.	0.	21 3F (4, 0) 38 3F (4, 4)
Γ_5	6958	6977	2.18	0.	34 3F (4, -1) 30 3F (4, 3)	Γ_5	6930		1.36	0.	38 3F (4, -1) 24 3F (4, 3)
Γ_3	7018		0.	0.	70 3F (4, 2) 26 1G (4, 2)	Γ_3	7009		0.	0.	70 3F (4, 2) 27 1G (4, 2)
Γ_1	9615		0.	0.	49 1G (4, 0) 33 3F (4, 0)	Γ_1	9588		0.	0.	54 1G (4, 0) 40 3F (4, 0)
Γ_5	9687	9682	3.62	0.	40 1G (4, 3) 25 3F (4, 3)	Γ_5	9622		4.18	0.	41 1G (4, 3) 30 3F (4, 3)
Γ_2	9873		0.	0.	64 1G (4, -4) 33 3F (4, -4)	Γ_2	9836		0.	0.	62 1G (4, -4) 35 3F (4, -4)
Γ_1	9921		0.	0.	54 1G (4, 4) 27 3F (4, 4)	Γ_1	9841		0.	0.	60 1G (4, 4) 34 3F (4, 4)
Γ_4	9946		0.	0.	66 1G (4, -2) 31 3F (4, -2)	Γ_4	9900		0.	0.	64 1G (4, -2) 33 3F (4, -2)
Γ_5	9956	9934	.72	0.	43 1G (4, -1) 21 3F (4, -1)	Γ_5	9902		.20	0.	45 1G (4, -1) 25 3F (4, -1)
Γ_3	10257		0.	0.	70 1G (4, 2) 27 3F (4, 2)	Γ_3	10269		0.	0.	69 1G (4, 2) 28 3F (4, 2)
Γ_3	16583		0.	0.	88 1D (2, 2) 7 3P (2, 2)	Γ_3	16589		0.	0.	88 1D (2, 2) 7 3P (2, 2)
Γ_5	16736	16740	-2.07	-.60	89 1D (2, -1) 8 3P (2, -1)	Γ_5	16759	16758	-2.07	0.	88 1D (2, -1) 8 3P (2, -1)
Γ_1	16793	16790	0.	0.	88 1D (2, 0) 8 3P (2, 0)	Γ_1	16802	16802	0.	0.	88 1D (2, 0) 9 3P (2, 0)
Γ_4	16944	16940	0.	0.	87 1D (2, -2) 9 3P (2, -2)	Γ_4	16908		0.	0.	86 1D (2, -2) 9 3P (2, -2)
Γ_1	20475	20475	0.	0.	98 3P (0, 0) 0 1S (0, 0)	Γ_1	20447	20452	0.	0.	98 3P (0, 0) 0 1S (0, 0)
Γ_5	21074	21061	-3.04	-3.20	99 3P (1, -1) 0 1I (6, -1)	Γ_5	21060	21048	-3.02	0.	99 3P (1, -1) 0 1I (6, -1)
Γ_2	21100	21084	0.	0.	69 3H (6, -4) 14 1I (6, -4)	Γ_2	21067		0.	0.	34 3P (1, 0) 36 3H (6, -4)
Γ_5	21151	21143	-5.64	-4.41	57 1I (6, -5) 30 1I (6, -1)	Γ_5	21098	21097	-5.64	0.	55 1I (6, -5) 33 1I (6, -1)
Γ_1	21154	21162	0.	0.	41 1I (6, 0) 57 1I (6, 4)	Γ_1	21106	21107	0.	0.	46 1I (6, 0) 51 1I (6, 4)
Γ_3	21253		0.	0.	86 1I (6, 2) 12 1I (6, 6)	Γ_3	21216		0.	0.	85 1I (6, 2) 12 1I (6, 6)
Γ_5	21297		-1.54	0.	43 1I (6, 3) 37 1I (6, -5)	Γ_5	21267		-1.79	0.	41 1I (6, 3) 38 1I (6, -5)
Γ_2	21324		0.	0.	60 1I (6, -4) 18 3P (1, 0)	Γ_2	21293		0.	0.	26 3P (1, 0) 46 3H (6, -4)
Γ_4	21391		0.	0.	93 1I (6, -6) 6 1I (6, -2)	Γ_4	21370		0.	0.	85 1I (6, -6) 13 1I (6, -2)
Γ_3	21428		0.	0.	87 1I (6, 6) 11 1I (6, 2)	Γ_3	21425		0.	0.	86 1I (6, 6) 11 1I (6, 2)
Γ_1	21574		0.	0.	56 1I (6, 0) 42 1I (6, 4)	Γ_1	21506		0.	0.	50 1I (6, 0) 47 1I (6, 4)
Γ_5	21596		1.18	0.	51 1I (6, -1) 44 1I (6, 3)	Γ_5	21525		1.42	0.	48 1I (6, 3) 45 1I (6, -1)
Γ_4	21631		0.	0.	88 1I (6, -2) 6 1I (6, -6)	Γ_4	21576		0.	0.	78 1I (6, -2) 13 1I (6, -6)
Γ_5	22207	22224	-2.88	0.	91 3P (2, -1) 8 1D (2, -1)	Γ_5	22206	22211	-2.89	0.	90 3P (2, -1) 8 1D (2, -1)
Γ_1	22221	22236	0.	0.	89 3P (2, 0) 9 1D (2, 0)	Γ_3	22208		0.	0.	89 3P (2, 2) 8 1D (2, 2)
Γ_3	22224		0.	0.	89 3P (2, 2) 8 1D (2, 2)	Γ_1	22229	22233	0.	0.	88 3P (2, 0) 9 1D (2, 0)
Γ_4	22301		0.	0.	85 3P (2, -2) 10 1D (2, -2)	Γ_4	22300		0.	0.	82 3P (2, -2) 10 1D (2, -2)
Γ_1	46024		0.	0.	99 1S (0, 0) 0 3P (0, 0)	Γ_1	45726		0.	0.	98 1S (0, 0) 0 3P (0, 0)

Table II

Nd ³⁺ :YPO ₄											Nd ³⁺ :LuPO ₄										
Sym	Energy (cm ⁻¹)		Splitting Factors				Eigenvector Composition				Sym	Energy (cm ⁻¹)		Splitting Factors				Eigenvector Composition			
			g		g _⊥		SLQ(2J, 2J _z)		SLQ(2J, 2J _z)					g		g _⊥		SLQ(2J, 2J _z)		SLQ(2J, 2J _z)	
	cal	obs	cal	obs	cal	obs	%	largest	%	second		cal	obs	cal	obs	cal	obs	%	largest	%	second
Γ ₇	0	0	3.00	3.09	1.36	1.22	67	4I (9, 7)	26	4I (9, -1)	Γ ₇	0	0	2.56	2.84	1.61	1.34	61	4I (9, 7)	32	4I (9, -1)
Γ ₇	107	99	-0.36		1.10		52	4I (9, -1)	26	4I (9, 7)	Γ ₇	120	120	.00		.80		46	4I (9, -1)	32	4I (9, 7)
Γ ₇	220		-5.49		1.07		77	4I (9, -9)	17	4I (9, -1)	Γ ₇	256		-5.44		1.12		76	4I (9, -9)	18	4I (9, -1)
Γ ₆	265		-1.30		2.74		75	4I (9, -3)	19	4I (9, 5)	Γ ₆	267		-1.19		2.83		73	4I (9, -3)	21	4I (9, 5)
Γ ₆	397		2.35		2.75		76	4I (9, 5)	19	4I (9, -3)	Γ ₆	413		2.23		2.84		74	4I (9, 5)	21	4I (9, -3)
Γ ₇	1984		-6.40		2.14		75	4I (11, -9)	21	4I (11, -1)	Γ ₇	1988		-5.31		3.02		62	4I (11, -9)	31	4I (11, -1)
Γ ₆	2019		-9.10		.75		80	4I (11,-11)	13	4I (11, -3)	Γ ₆	2030		-5.52		2.53		46	4I (11,-11)	36	4I (11, -3)
Γ ₇	2043		-1.36		1.79		59	4I (11, -1)	21	4I (11, -9)	Γ ₇	2049		-2.12		.54		46	4I (11, -1)	33	4I (11, -9)
Γ ₆	2059		-1.74		4.50		50	4I (11, -3)	31	4I (11, 5)	Γ ₆	2065		-5.02		2.77		49	4I (11,-11)	24	4I (11, -3)
Γ ₇	2133		5.42		1.62		79	4I (11, 7)	17	4I (11, -1)	Γ ₇	2143		5.10		1.99		76	4I (11, 7)	20	4I (11, -1)
Γ ₆	2157		2.22		5.27		64	4I (11, 5)	33	4I (11, -3)	Γ ₆	2168		1.92		5.32		61	4I (11, 5)	35	4I (11, -3)
Γ ₆	3927	3931	-11.17		.45		91	4I (13,-11)	6	4I (13, -3)	Γ ₆	3931		-10.47		.92		85	4I (13,-11)	11	4I (13, -3)
Γ ₇	3970	3973	-1.60		7.23		80	4I (13, -1)	12	4I (13, -9)	Γ ₇	3960	3964	-1.58		7.20		78	4I (13, -1)	13	4I (13, -9)
Γ ₆	4003	4005	9.48		1.44		63	4I (13, 13)	16	4I (13, -3)	Γ ₆	4004	4005	3.35		3.30		34	4I (13, -3)	27	4I (13, 13)
Γ ₆	4029	4030	3.00		4.38		52	4I (13, -3)	31	4I (13, 13)	Γ ₆	4039	4037	8.42		2.13		65	4I (13, 13)	28	4I (13, -3)
Γ ₇	4066	4066	-8.45		1.68		84	4I (13, -9)	9	4I (13, -1)	Γ ₇	4069	4073	-8.07		2.26		82	4I (13, -9)	9	4I (13, -1)
Γ ₆	4142	4157	3.71		6.28		72	4I (13, 5)	22	4I (13, -3)	Γ ₆	4148	4131	3.74		6.36		68	4I (13, 5)	24	4I (13, -3)
Γ ₇	4150	4159	6.89		2.00		88	4I (13, 7)	9	4I (13, -1)	Γ ₇	4153	4166	6.49		2.59		85	4I (13, 7)	11	4I (13, -1)
Γ ₆	5829	5829	15.17		.24		95	4I (15, 13)	1	4I (15, 5)	Γ ₆	5828	5831	14.96		.48		93	4I (15, 13)	3	4I (15, 5)
Γ ₇	5922	5924	-1.12		9.42		93	4I (15, -1)	2	4I (15, -9)	Γ ₇	5906		-1.14		9.39		92	4I (15, -1)	3	4I (15, -9)
Γ ₆	5986		-8.58		1.32		54	4I (15,-11)	41	4I (15, -3)	Γ ₆	5966		-8.13		1.18		50	4I (15,-11)	43	4I (15, -3)
Γ ₆	6092		-6.91		4.23		46	4I (15, -3)	43	4I (15,-11)	Γ ₆	6094		-6.98		4.56		46	4I (15,-11)	41	4I (15, -3)
Γ ₇	6162		17.38		.09		93	4I (15, 15)	5	4I (15, 7)	Γ ₇	6174		16.77		.29		87	4I (15, 15)	9	4I (15, 7)
Γ ₆	6243	6243	4.86		5.79		85	4I (15, 5)	10	4I (15, -3)	Γ ₆	6243	6250	4.68		6.23		82	4I (15, 5)	12	4I (15, -3)
Γ ₇	6262		-10.29		2.08		93	4I (15, -9)	2	4I (15, -1)	Γ ₇	6258		-9.95		2.14		92	4I (15, -9)	2	4I (15, -1)
Γ ₇	6321	6314	8.35		2.25		89	4I (15, 7)	5	4I (15, 15)	Γ ₇	6324	6324	8.65		2.53		83	4I (15, 7)	9	4I (15, 15)
Γ ₇	11409	11410	-0.51	-0.44	.79	.86	93	4F (3, -1)	4	2D1(3, -1)	Γ ₇	11410	11410	-0.48	-0.49	.81	.80	93	4F (3, -1)	4	2D1(3, -1)
Γ ₆	11457	11461	-1.35	-0.90	.23		93	4F (3, -3)	4	2D1(3, -3)	Γ ₆	11439	11443	-1.29	-1.12	.27	.15	93	4F (3, -3)	4	2D1(3, -3)
Γ ₆	12433	12444	.21		1.33		57	4F (5, -3)	19	2H2(9, 5)	Γ ₆	12418	12422	-0.59		2.14		67	4F (5, -3)	12	4F (5, 5)
Γ ₇	12435	12434	-1.64		2.73		88	4F (5, -1)	2	2H2(9, -9)	Γ ₇	12425	12422	-1.80		2.73		85	4F (5, -1)	4	2H2(9, -9)
Γ ₆	12453	12450	3.30		.62		29	4F (5, 5)	24	2H2(9, 5)	Γ ₆	12453	12451	4.75		1.16		32	2H2(9, 5)	31	4F (5, 5)
Γ ₆	12495		-2.59		1.01		48	2H2(9, -3)	12	4F (9, -3)	Γ ₆	12504	12507	-1.89		.28		45	2H2(9, -3)	13	4F (5, 5)

Γ_6	12526	12520	3.31	2.74	1.40	1.23	60 4F (5, 5)	20 4F (5, -3)	Γ_6	12521	1.92	.33	38 4F (5, 5)	29 4F (5, -3)			
Γ_6	12564	12583	-7.56		.70		44 2H2(9, -9)	10 4F (9, -9)	Γ_7	12557	12577	-7.56	.55	44 2H2(9, -9)	10 4F (9, -9)		
Γ_7	12617		-1.77		3.90		45 2H2(9, -1)	11 4F (9, -1)	Γ_7	12630		-1.20	3.74	45 2H2(9, -1)	11 4F (9, -1)		
Γ_7	12670		6.55		.45		52 2H2(9, 7)	12 4F (9, 7)	Γ_7	12673		6.13	.79	50 2H2(9, 7)	12 4F (9, 7)		
Γ_7	13367	13369	-.77	-.81	4.60	4.37	91 4F (7, -1)	4 2G1(7, -1)	Γ_7	13364	13366	-.77	4.61	91 4F (7, -1)	3 2G1(7, -1)		
Γ_6	13382	13385	5.87	5.47	1.29	1.22	89 4F (7, 5)	3 2G1(7, 5)	Γ_6	13368	13369	5.76	5.57	88 4F (7, 5)	3 2G1(7, 5)		
Γ_7	13484	13479	8.29		.06		90 4F (7, 7)	3 2G1(7, 7)	Γ_7	13457	13449	8.29	.05	90 4F (7, 7)	3 2G1(7, 7)		
Γ_6	13487	13484	-3.43		1.11		89 4F (7, -3)	4 2G1(7, -3)	Γ_6	13485	13482	-3.32	1.35	88 4F (7, -3)	4 2G1(7, -3)		
Γ_7	13520	13515	-1.78	-1.82	3.85		92 4S (3, -1)	4 2P (3, -1)	Γ_6	13504	13505	-5.85	-5.86	.01	93 4S (3, -3)	4 2P (3, -3)	
Γ_6	13522	13517	-5.86	-5.85	.01		93 4S (3, -3)	4 2P (3, -3)	Γ_7	13505	13505	-1.80	-1.95	3.86	92 4S (3, -1)	4 2P (3, -1)	
Γ_7	14635	14635	-.42		5.57		58 4F (9, -1)	15 2H2(9, -1)	Γ_7	14622		-.29	5.32	50 4F (9, -1)	15 4F (9, 7)		
Γ_6	14639	14638	-.15		5.35		46 4F (9, -3)	27 4F (9, 5)	Γ_6	14623	14624	.31	5.45	43 4F (9, -3)	31 4F (9, 5)		
Γ_7	14720	14726	-1.38		3.58		37 4F (9, -9)	36 4F (9, 7)	Γ_7	14697	14702	-4.07	3.52	48 4F (9, -9)	26 4F (9, 7)		
Γ_7	14740		-1.96		4.17		33 4F (9, -9)	26 4F (9, 7)	Γ_7	14730		.61	4.36	32 4F (9, 7)	23 4F (9, -1)		
Γ_6	14741	14759	2.43		5.42		46 4F (9, 5)	27 4F (9, -3)	Γ_6	14739	14747	1.95	5.53	43 4F (9, 5)	31 4F (9, -3)		
Γ_7	15846		-1.81		6.14		71 2H2(11, -1)	11 2H1(11, -1)	Γ_7	15842		-3.58	4.97	55 2H2(11, -1)	22 2H2(11, -9)		
Γ_7	15857		-9.11		.52		72 2H2(11, -9)	11 2H1(11, -9)	Γ_7	15851		-7.32	1.74	56 2H2(11, -9)	22 2H2(11, -1)		
Γ_6	15877		-4.24		1.53		67 2H2(11, -3)	11 2H1(11, -3)	Γ_6	15872		-5.40	1.27	57 2H2(11, -3)	20 2H2(11, -11)		
Γ_7	15890	15898	7.71		.10		78 2H2(11, 7)	12 2H1(11, 7)	Γ_7	15882	15884	7.70	.16	3.62	78 2H2(11, 7)	12 2H1(11, 7)	
Γ_6	15898		-10.35		.86		67 2H2(11, -11)	10 2H1(11, -11)	Γ_6	15892		-9.06	1.43	57 2H2(11, -11)	17 2H2(11, -3)		
Γ_6	15905		4.76		2.40		74 2H2(11, 5)	11 2H1(11, 5)	Γ_6	15901		4.64	2.72	73 2H2(11, 5)	11 2H1(11, 5)		
Γ_6	16989	16980	.64	.80	.04	.61	61 4G (5, -3)	22 4G (5, 5)	Γ_6	16955	16950	.81	.86	.19	.63	59 4G (5, -3)	26 4G (5, 5)
Γ_7	17061	17059	-.23	.35	.06	.26	65 4G (5, -1)	8 4G (7, 7)	Γ_7	17035	17035	-.07	.41	.24	.54	67 4G (5, -1)	8 4G (7, 7)
Γ_6	17096	17109	-.67		.31	.37	30 4G (5, 5)	28 4G (7, -3)	Γ_6	17082		-.80	.19			29 4G (7, -3)	26 4G (5, 5)
Γ_7	17189		2.83		1.87		20 4G (7, 7)	18 4G (7, -1)	Γ_7	17182		2.45	2.05			20 4G (7, -1)	18 4G (7, 7)
Γ_6	17216	17205	2.42	2.39	1.33	1.23	28 4G (5, 5)	20 4G (7, 5)	Γ_6	17203	17191	2.25	1.52			27 4G (5, 5)	20 4G (7, 5)
Γ_7	17265		2.47		.29		32 4G (5, -1)	12 4G (7, 7)	Γ_7	17263		2.67	.30			30 4G (5, -1)	13 4G (7, 7)
Γ_6	17274		.81		1.66		32 4G (5, -3)	15 4G (5, 5)	Γ_6	17280		.93	1.60			32 4G (5, -3)	16 4G (5, 5)
Γ_6	18864	18885	-2.78	-3.05	1.50	.98	52 4G (7, -3)	20 2G1(7, -3)	Γ_6	18839	18860	-2.72	-2.73	1.67	1.34	50 4G (7, -3)	19 2G1(7, -3)
Γ_7	18942		1.10		2.61		42 4G (7, -1)	14 2G1(7, -1)	Γ_7	18908		1.42	2.45			38 4G (7, -1)	16 4G (7, 7)
Γ_6	18955	18957	4.63	4.48	1.69	1.25	50 4G (7, 5)	16 2G1(7, 5)	Γ_6	18934	18934	4.56	4.32	1.89	1.36	48 4G (7, 5)	16 2G1(7, 5)
Γ_7	19035	19023	4.66	4.73	.97	1.10	43 4G (7, 7)	17 2G1(7, 7)	Γ_7	19015	18997	4.33	4.01	1.11	1.34	41 4G (7, 7)	16 4G (7, -1)
Γ_7	19295		-1.70		4.63		25 4G (9, -1)	18 2K (13, -1)	Γ_7	19244		-.73	5.13			25 2K (13, -1)	21 4G (9, -1)
Γ_6	19317		10.44		.13		78 2K (13, 13)	8 4G (9, 5)	Γ_6	19296	19296	.06	4.43			39 2K (13, 5)	34 2K (13, -3)
Γ_6	19352		-.68		1.86		30 2K (13, 5)	23 2K (13, -3)	Γ_6	19338		8.55	1.66			58 2K (13, 13)	20 4G (9, 5)
Γ_7	19356		-6.65		1.92		47 4G (9, -9)	10 2K (13, -9)	Γ_7	19341		-7.19	1.69			49 4G (9, -9)	12 2K (13, -9)
Γ_7	19392		6.08		1.18		57 4G (9, 7)	7 2G1(9, 7)	Γ_7	19376		5.66	1.50			54 4G (9, 7)	7 2G1(9, 7)
Γ_6	19421		-1.90		3.67		58 4G (9, -3)	6 4G (9, 5)	Γ_6	19400	19400	-1.93	2.85			60 4G (9, -3)	5 2K (13, -3)
Γ_6	19449		.61		2.80		30 4G (9, 5)	23 2K (13, -11)	Γ_7	19420		.35	4.86			40 4G (9, -1)	15 2K (13, -1)
Γ_7	19456		.94		4.53		31 4G (9, -1)	29 2K (13, 7)	Γ_6	19440		3.10	2.58			26 4G (9, 5)	17 2K (13, -3)

Γ_6 19493	-2.62	2.85	46 2K (13, -11)	19 2K (13, 5)	Γ_6 19484	-2.92	2.20	52 2K (13, -11)	18 2K (13, 5)
Γ_7 19524	-2.46	3.25	34 2K (13, 7)	34 2K (13, -9)	Γ_7 19499	-.91	3.00	42 2K (13, 7)	25 2K (13, -9)
Γ_6 19587	.12	5.58	42 2K (13, -3)	36 2K (13, 5)	Γ_6 19563	-.88	5.10	36 2K (13, -3)	29 2K (13, 5)
Γ_7 19606	-2.60	5.36	49 2K (13, -1)	29 2K (13, -9)	Γ_7 19582	-3.56	4.81	39 2K (13, -1)	37 2K (13, -9)
Γ_7 20872	5.67	1.33	22 2G1(9, 7)	15 4G (9, 7)	Γ_7 20841	5.80	1.24	22 2G1(9, 7)	15 4G (9, 7)
Γ_6 20886	.43	5.02	19 2G1(9, -3)	15 2G1(9, 5)	Γ_6 20857	.72	5.05	17 2G1(9, -3)	16 2G1(9, 5)
Γ_7 20934 20944	1.00	3.47	24 2G1(9, -1)	16 4G (9, -1)	Γ_7 20913 20911	.62	3.29	23 2G1(9, -1)	14 4G (9, -1)
Γ_6 20962 20931	1.92	4.96	19 2G1(9, 5)	14 2G1(9, -3)	Γ_6 20942 20924	1.69	5.00	17 2G1(9, 5)	15 2G1(9, -3)
Γ_7 21028	-9.64	.02	35 2G1(9, -9)	22 2G2(9, -9)	Γ_7 20990	-9.44	.12	34 2G1(9, -9)	21 2G2(9, -9)
Γ_7 21090	-1.40	2.65	34 2D1(3, -1)	29 2P (3, -1)	Γ_7 21060	-1.18	2.89	31 2D1(3, -1)	27 2P (3, -1)
Γ_6 21142 21144	-3.37 -3.09	.13	41 2D1(3, -3)	35 2P (3, -3)	Γ_6 21106 21112	-3.41	.24	39 2D1(3, -3)	34 2P (3, -3)
Γ_7 21235	-2.26	5.33	38 4G (11, -1)	25 4G (11, -9)	Γ_7 21194	-1.50	5.46	41 4G (11, -1)	17 4G (11, -9)
Γ_6 21305	.54	5.93	47 4G (11, -3)	34 4G (11, 5)	Γ_6 21256	.80	5.05	43 4G (11, -3)	32 4G (11, 5)
Γ_7 21313	2.95	2.49	36 2K (15, 15)	35 4G (11, -9)	Γ_6 21292 21293	-3.10	4.73	23 2K (15, -3)	21 2K (15, -11)
Γ_7 21337	4.53	2.74	36 2K (15, 15)	16 4G (11, -9)	Γ_7 21292	-6.26	.09	53 4G (11, -9)	10 2K (15, -1)
Γ_6 21338 21319	-1.88	5.42	24 2K (15, -11)	20 2K (15, 13)	Γ_7 21335	8.54	1.68	47 2K (15, 15)	11 4G (11, 7)
Γ_6 21382	2.76	4.03	45 2K (15, 13)	16 4G (11, -11)	Γ_6 21377	1.51	3.46	35 2K (15, 13)	21 4G (11, -11)
Γ_7 21438	-3.55	4.54	42 2K (15, -9)	16 2K (15, -1)	Γ_7 21406	1.20	2.85	25 2K (15, 15)	24 2K (15, -9)
Γ_6 21474	-2.48	2.76	28 4G (11, -11)	25 2K (15, -3)	Γ_6 21445	-1.86	.82	31 4G (11, -11)	21 2K (15, -3)
Γ_7 21496	4.17	.65	38 2K (15, 7)	20 4G (11, 7)	Γ_7 21475	3.03	3.33	51 2K (15, 7)	14 2K (15, -9)
Γ_6 21513	-2.24	1.25	34 2K (15, 5)	20 2K (15, -11)	Γ_6 21487	.07	.78	39 2K (15, 5)	16 2K (15, -11)
Γ_7 21539	3.11	1.93	29 4G (11, 7)	22 2K (15, -9)	Γ_7 21524	3.47	.91	35 4G (11, 7)	18 2K (15, -9)
Γ_6 21555	-5.00	1.37	22 2K (15, -11)	17 4G (11, -3)	Γ_6 21533	-6.52	2.73	34 2K (15, -11)	27 2K (15, -3)
Γ_6 21583	1.28	.98	26 4G (11, 5)	23 2K (15, -3)	Γ_6 21570	2.07	4.66	44 4G (11, 5)	30 4G (11, -3)
Γ_7 21608	.07	7.02	45 2K (15, -1)	18 2K (15, 7)	Γ_7 21575	.37	6.54	37 2K (15, -1)	16 2K (15, 7)
Γ_7 23170 23154	-.60 -.75	.63	92 2P (1, -1)	7 4D (1, -1)	Γ_7 23143 23129	-.61 -.92	.63	92 2P (1, -1)	7 4D (1, -1)
Γ_7 23657	-1.18	3.57	96 2D1(5, -1)	2 4F (5, -1)	Γ_7 23659	-1.19	3.58	96 2D1(5, -1)	2 4F (5, -1)
Γ_6 23679	-3.15	1.10	92 2D1(5, -3)	4 2D1(5, 5)	Γ_6 23664	-2.40	1.77	84 2D1(5, -3)	11 2D1(5, 5)
Γ_6 23757	5.57	1.11	92 2D1(5, 5)	4 2D1(5, -3)	Γ_6 23719	4.81	1.78	85 2D1(5, 5)	11 2D1(5, -3)
Γ_7 26104	-1.10	2.18	51 2P (3, -1)	41 2D1(3, -1)	Γ_7 26076	-1.10	2.18	51 2P (3, -1)	40 2D1(3, -1)
Γ_6 26148	-3.28	.00	51 2P (3, -3)	40 2D1(3, -3)	Γ_6 26095	-3.28	0.	51 2P (3, -3)	40 2D1(3, -3)
Γ_6 27805 27804	-.55 -.13	2.16	53 4D (3, -3)	17 4D (5, 5)	Γ_6 27771 27773	-.19 .20	2.28	50 4D (3, -3)	20 4D (5, 5)
Γ_7 27892 27906	-.45 -1.86	2.15	80 4D (3, -1)	13 2D2(3, -1)	Γ_7 27857 27865	-.67 -1.29	2.19	80 4D (3, -1)	13 2D2(3, -1)
Γ_6 28045 28044	1.18	.34	41 4D (5, 5)	27 4D (3, -3)	Γ_6 27996 27996	-1.35	.88	29 4D (3, -3)	25 4D (5, -3)
Γ_7 28078	-1.60	4.05	78 4D (5, -1)	17 2D2(5, -1)	Γ_7 28029 28030	-1.47	4.04	79 4D (5, -1)	17 2D2(5, -1)
Γ_6 28168 28172	-1.34	2.42	58 4D (5, -3)	20 4D (5, 5)	Γ_6 28140 28143	.82	3.05	44 4D (5, -3)	34 4D (5, 5)
Γ_7 28454 28442	-.35	.14	89 4D (1, -1)	7 2P (1, -1)	Γ_7 28408 28401	-.25	.10	90 4D (1, -1)	7 2P (1, -1)
Γ_7 29018 29032	.15	4.55	34 2I (11, 7)	23 2I (11, -9)	Γ_7 28932	.81	4.56	34 2I (11, 7)	29 2I (11, -1)
Γ_6 29031	-1.41	4.26	32 2I (11, 5)	31 2I (11, -3)	Γ_6 28933	-.28	4.81	35 2I (11, 5)	35 2I (11, -3)

Γ_7 29094	-2.77	3.98	50 2I (11, -9) 30 2I (11, 7)	Γ_7 29042	-3.36	3.89	53 2I (11, -9) 27 2I (11, 7)
Γ_6 29115	-6.69	.75	61 2I (11,-11) 18 2I (11, 5)	Γ_6 29067	-7.59	.07	66 2I (11,-11) 14 2I (11, 5)
Γ_7 29291	-.05	5.18	55 2I (11, -1) 15 2I (11, 7)	Γ_7 29224	-.10	5.08	48 2I (11, -1) 18 2I (11, 7)
Γ_6 29309	-.30	4.94	47 2I (11, -3) 30 2I (11, 5)	Γ_6 29241	-.50	4.82	43 2I (11, -3) 30 2I (11, 5)
Γ_7 29722	13.99	.01	93 2L (15, 15) 4 2K (15, 15)	Γ_7 29719	13.90	.05	92 2L (15, 15) 4 2K (15, 15)
Γ_7 29931	-7.54	2.44	85 2L (15, -9) 5 2L (15, -1)	Γ_7 29838	-.01	6.54	43 2L (15, 7) 33 2L (15, -9)
Γ_7 29948	5.56	2.34	85 2L (15, 7) 4 2L (15, -9)	Γ_7 29845	-1.97	6.44	53 2L (15, -9) 40 2L (15, 7)
Γ_6 29982	1.45	6.14	60 2L (15, 5) 23 2L (15, -3)	Γ_6 29860	2.45	6.57	65 2L (15, 5) 27 2L (15, -3)
Γ_6 30002	-4.72	3.91	66 2L (15,-11) 16 2L (15, 13)	Γ_6 29933	-8.43	2.24	79 2L (15,-11) 6 2L (15, -3)
Γ_6 30015	8.55	3.63	74 2L (15, 13) 12 2L (15,-11)	Γ_6 29978	11.24	1.76	88 2L (15, 13) 4 2K (15, 13)
Γ_7 30093	9.43	.21	93 4D (7, 7) 3 4D (7, -1)	Γ_6 30027	-1.45	6.02	58 2L (15, -3) 20 2L (15, 5)
Γ_6 30123	4.01	3.95	70 4D (7, 5) 18 4D (7, -3)	Γ_7 30072	.26	6.58	67 2L (15, -1) 8 4D (7, 7)
Γ_6 30142 30141	-.88	5.84	61 2L (15, -3) 19 2L (15, 5)	Γ_6 30073	2.96	4.70	61 4D (7, 5) 34 4D (7, -3)

Table III: Semiempirical Hamiltonian Paramters

Ion:	Pr ³⁺		Nd ³⁺		Er ^{3+c}	
	YPO ₄	LuPO ₄	YPO ₄	LuPO ₄	YPO ₄	LuPO ₄
Param.						
ξ_{4f}	739.0(14)	743.6(21)	880.1(11)	877.5(9)	2367.8(47)	2366.5(18)
F^2	67778(675)	67687(54)	72287(53)	71804(380)	97058(103)	97015(93)
F^4	49603(1780)	48633(426)	52688(1537)	52128(1029)	69142(194)	69141(92)
F^6	32413(64)	32151(190)	36839(1738)	36035(1149)	48232(199)	48232(158)
B_0^2	78(18)	21(50)	302(33)	178(25)	279(52)	146(51)
B_0^4	321(51)	280(48)	273(53)	209(42)	155(99)	69(78)
B_4^4	-849(43)	-808(125)	-777(43)	-922(25)	-756(56)	-760(44)
B_0^6	-1376(67)	-1658(102)	-1245(38)	-1256(38)	-537(58)	-643(41)
B_4^6	35(41)	291(133)	-109(57)	-147(51)	-141(48)	-89(40)
α	21.2(1)	21.2 ^a	19.6(3)	18.9(3)	15.9 ^b	15.9 ^b
β	-665(17)	-665 ^a	-600(10)	-581(11)	-632 ^b	-632 ^b
γ	1534(632)	1534 ^a	1083(539)	1280(358)	2017 ^b	2017 ^b
M^0	1.76 ^b	1.76 ^b	2.24 ^b	2.24 ^b	4.50 ^b	4.50 ^b
M^4	0.99 ^b	0.99 ^b	1.25 ^b	1.25 ^b	2.52 ^b	2.52 ^b
M^6	0.67 ^b	0.67 ^b	0.84 ^b	0.84 ^b	1.71 ^b	1.71 ^b
P^2	275 ^b	275 ^b	213 ^b	213 ^b	667 ^b	667 ^b
P^4	206 ^b	206 ^b	160 ^b	160 ^b	500.3 ^b	500.3 ^b
P^6	138 ^b	138 ^b	106 ^b	106 ^b	333.5 ^b	333.5 ^b
T^2			306 ^b	306 ^b	157.5 ^b	157.5 ^b
T^3			41 ^b	41 ^b	48 ^b	48 ^b
T^4			59 ^b	59 ^b	18 ^b	18 ^b
T^6			-283 ^b	-283 ^b	-342 ^b	-342 ^b
T^7			326 ^b	326 ^b	214 ^b	214 ^b
T^8			298 ^b	298 ^b	449 ^b	449 ^b
σ	14.7	27.3	11.4	9.1	14.7	13.2

^aFixed at Pr³⁺:YPO₄ value

^bFrom reference 11

^cFrom reference 8

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