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Correlation-crystal-field delta-function analysis of $4f^2$ (Pr^{3+}) energy-level structure

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Abstract

Standard formulations of the electronic energy-level Hamiltonian, applied to lanthanide systems, have been used with great success in rationalizing observed energy-level splittings and Stark level orderings. However, these standard models do not satisfactorily account for the energy-level structures observed for specific anomalous multiplet manifolds, such as the $^1D_2$ multiplet of Pr^{3+}. In the present study, we apply a simplified correlation-crystal-field model to the $4f^2$ electronic energy-level structure of Pr^{3+} in seven different crystalline hosts. This highly restricted form of the correlation-crystal-field (CCF) contribution to the model energy-level Hamiltonian, called the 'δ-function' CCF model, considers two-electron correlation effects only from paired electrons within the same angular orbital, an assumption that reduces the plethora of applicable CCF operators to only two important independent terms. When the 'δ-function' CCF model is applied to the electronic energy-level structures of $LaCl_3$:Pr^{3+}, $GdCl_3$:Pr^{3+}, $Cs_2NaPrCl_6$, Cs_2NaYCl_6:Pr^{3+}, $LiYF_4$:Pr^{3+}, $LiBiF_4$:Pr^{3+}, and $CsCdBr_3$:Pr^{3+}, the major discrepancies between observed and calculated crystal-field splittings in the $^1D_2$ multiplet manifold for each system are successfully resolved. © 1998 Elsevier Science S.A.

Keywords: Correlation-crystal-field; Delta-function; Energy-level modeling; Praseodymium

1. Introduction

An enormous amount of effort has been devoted to measurements and analyses of the $4f^N$ electronic state structures of trivalent lanthanide ions (Ln^{3+}) in crystals. Model Hamiltonians, constructed to represent the principal interactions that contribute to $4f^N$ (Ln^{3+}) state structure, have been used with great success in rationalizing the energy-level structures of these systems. However, these 'standard models' do not satisfactorily account for the crystal-field energy-level splittings and Stark level orderings observed within specific anomalous $4f^N[SL]J$ multiplet manifolds, even under conditions in which the crystal-field energy-level structures of all the remaining multiplet manifolds are well explained by standard modeling calculations. For any given Ln^{3+} ion, the identities of the problematic multiplet manifolds persist from host system to host system. Among these problematic multiplet manifolds, the greatest attention has focused on the $^2H_{11/2}$, $^2H_{9/2}$, $^2G_{9/2}$, and $^2G_{7/2}$ multiplets of $Nd^{3+}(4f^3)$ [1–5] and $Er^{3+}(4f^{11})$ [6,7], and on the $^1D_2$ and $^1G_4$ multiplets of $Pr^{3+}(4f^2)$ [8–11] and $Tm^{3+}(4f^{12})$ [12].

In 'standard' models, the model Hamiltonian is generally partitioned into an isotropic atomic-like part, $\mathbf{H}_a$, that largely determines the baricenter energies and SL compositions of the $4f^N[SL]J$ multiplets, and an anisotropic crystal-field interaction part, $\mathbf{H}_{cf}$, that determines the JM_J compositions and relative energies of the Stark levels split out of the various J-multiplet manifolds. The extant formulations of the $\mathbf{H}_a$ operator used in most $4f^N$ energy-level modeling calculations are quite adequate for representing the major contributions to the LS (term) and $[SL]J$ (multiplet) structures observed for most $Ln^{3+}(4f^N)$ systems. Similarly, the one-electron crystal-field operators, $\mathbf{H}_{cf}$, used in standard modeling calculations, generally give a reasonably good account of Stark level splittings observed within the great majority of J-multiplet manifolds. However, these standard modeling calculations persistently fail to account for the observed crystal-field energy-level structures for a number of specific multiplets. Often these recalcitrant multiplets are simply ignored in performing energy-level analyses and in making detailed assignments of optical line spectra. This is highly unsatisfactory from a theoretical point of view, and it is also an unattractive

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option in cases where the neglected multiplets are known or suspected to have properties of significant practical interest. Consequently, there is considerable interest in identifying how the standard crystal-field interaction models may be augmented to deal with the problematic multiplet manifolds.

Several approaches have been used in addressing the problematic multiplets. In one approach, the anisotropic crystal-field interaction Hamiltonian is augmented to include two-electron f^N/correlation-crystal-field (CCF) interaction terms [13–16] as well as the standard one-electron crystal-field (CF) interaction terms. The two-electron CCF operators in the augmented crystal-field Hamiltonian are defined to act only on 4f electrons, and the overall model Hamiltonian remains an intraconfigurational ($4f^N$) operator. This CCF approach to improving $4f^N$ crystal-field energy-level calculations and analyses has been applied with considerable success to a number of Ln^{3+} ($4f^N$) systems, and it has proved especially effective in dealing with the problematic multiplets of $Nd^{3+}(4f^3)$ and $Er^{3+}(4f^{11})$ systems. The major problem encountered in using this approach is in selecting which of the many possible CCF interaction terms should be included in the augmented crystal-field Hamiltonian. Even for systems where the Ln^{3+} site symmetry is very high (e.g. O_h), the total number of symmetry-allowed CCF interaction terms is much greater than can be dealt with in any meaningful and practical way. Therefore, considerable effort has been devoted to identifying which CCF interaction terms may be expected to make the largest contributions to the $4f^N$ energy-level structure of any given Ln^{3+} ion. From the calculations and analyses carried out on Nd^{3+} and Er^{3+} systems, it appears that only a few CCF interaction terms are needed to resolve the most serious discrepancies between calculated and observed crystal-field splittings in the problematic multiplet manifolds. Moreover, the same terms appear important for Nd^{3+} and Er^{3+} in a variety of crystalline hosts.

An alternative strategy that has been used in dealing with the problematic multiplet issue invokes crystal-field-induced *interconfigurational* mixing effects. In modeling calculations based on this strategy, the crystal-field Hamiltonian is expanded to include odd-parity interaction terms (where symmetry allows) as well as even-parity interaction terms, and it is treated as both an *intraconfigurational* and *interconfigurational* interaction operator. As an intraconfigurational operator, its actions are identical to those of the $\mathbf{H}_{cf}$ operator used in the standard crystal-field energy-level modeling calculations. However, as an interconfigurational interaction operator, it produces mixings between $4f^N$ and higher-energy configurations, with consequent alterations in the energy-level structures predicted by the standard calculations. Systematic applications of the crystal-field-induced configuration–interaction model pose major computational difficulties, and the importance of this model to understanding crystal-field energy-level structure remains unclear. However, this model has been applied with success in resolving disagreements between calculated versus observed crystal-field splittings in the $^1D_2$ multiplet of $Pr^{3+}(4f^2)$ in $PrCl_3$ [9,10] and in $LiYF_4$ [11].

In the present work, we apply a highly restricted form of the CCF interaction model to the $4f^2$ electronic energy-level structure of Pr^{3+} in seven different crystalline hosts. The Pr^{3+} site symmetries represented among these systems are C_{3h} in $LaCl_3{:}Pr^{3+}$ [17] and $GdGl_3{:}Pr^{3+}$ [18], where the lanthanide ion is coordinated to nine nearest neighbor Cl^- ions; O_h in $Cs_2NaPrCl_6$ and $Cs_2NaYCl_6{:}Pr^{3+}$ [19], where the lanthanide ion is coordinated to six nearest neighbor Cl^- ions; S_4 in $LiYF_4{:}Pr^{3+}$ and $LiBiF_4{:}Pr^{3+}$ [20], where the lanthanide ion is coordinated to eight F^- ions; and C_{3v} in $CsCdBr_3{:}Pr^{3+}$ [21], where the lanthanide ion is coordinated to six Br^- ions. In each of these systems, crystal-field splittings observed within the $^1D_2$ multiplet manifold of $4f^2$ (Pr^{3+}) are very poorly represented by calculations based on standard, one-electron crystal-field interaction models. Similar disagreements between observed and calculated crystal-field splittings are also found within the $^1G_4$ multiplet, but in most of the systems examined here, this multiplet manifold remains incompletely characterized with respect to the locations and symmetry assignments of Stark levels.

2. CCF δ-function

The CCF interaction model employed here derives directly from a model originally proposed by Judd [22], and more recently examined and developed by Lo and Reid [23]. This model is based on the assumption that the most important contributions to the CCF Hamiltonian may be represented by point-localized lanthanide–ligand interactions of the form

$$I_L = -A_L \delta(r_i - R_L)\delta(r_j - R_L) \tag{1}$$

where A_L is a positive constant, $\delta(r_i - R_L)$ and $\delta(r_j - R_L)$ are delta functions in which r_i and r_j are the coordinates of two f electrons (labeled i and j) and R_L denotes the coordinates of a point located on the lanthanide–ligand axis. For obvious reasons, this model is often referred to as the CCF 'δ-function' model, and many of its formal transformation properties and other attributes are discussed in a recent paper by McAven et al. [24]. Since Eq. (1) requires that the two electrons occupy the same point in space, correlation effects in this model are considered only from paired electrons in the same angular orbital (with opposite spin). Since these paired electrons have a much larger overlap function than does two unpaired electrons, this may be a reasonable assumption. In parametrized form, the CCF 'δ-function' Hamiltonian may be written as,

$$\boldsymbol{H}_{\mathrm{ccf}(\delta)} = \sum_{k,q} D^{k}_{q} \delta^{(k)}_{q} \tag{2}$$

where k runs over the even integers from 0 to 12, and allowed values of q are determined by the site symmetry. Contributions from $k=0$ are isotropic, and thus are already incorporated in the atomic Hamiltonian, $\mathbf{H}_{\mathrm{a}}$. In practice, contributions to the $\mathbf{H}_{\mathrm{ccf}(\delta)}$ operator from $k \geq 6$ terms are not found to be statistically significant, and thus may be neglected. This leaves only two significant terms, D^{2}_{q} and D^{4}_{q}, with respective operators given by,

$$\delta^{(2)}_{q} = \frac{35\sqrt{7}}{3\sqrt{2}} \mathbf{g}^{(2)}_{2q} - \frac{35\sqrt{7}}{\sqrt{22}} \mathrm{g}^{(2)}_{3q} - \frac{28\sqrt{105}}{\sqrt{143}} \mathrm{g}^{(2)}_{10q} \tag{3}$$

and

$$\delta^{(4)}_{q} = -\frac{21\sqrt{105}}{2\sqrt{11}} \mathrm{g}^{(4)}_{2q} + \frac{63\sqrt{105}}{22} \mathrm{g}^{(4)}_{3q} + \frac{84\sqrt{42}}{\sqrt{715}} \mathrm{g}^{(4)}_{10\mathrm{A}q} + \frac{8232\sqrt{3}}{11\sqrt{1105}} \mathrm{g}^{(4)}_{10\mathrm{B}q} \tag{4}$$

where the $\mathbf{g}^{(k)}_{\mathrm{i}q}$ are the orthogonal CCF operators of Judd [14] and Reid [15].

As can be seen from Eq. (3) and Eq. (4), the CCF δ-function model Hamiltonian contains only a small subset of the complete set of orthogonal CCF interaction operators encompassed in the general CCF Hamiltonian. However, included in this subset are contributions from all the terms found to make significant contributions to the crystal-field splittings observed in the problematic multiplet manifolds of $\mathrm{Nd}^{3+}(4f^3)$ and $\mathrm{Er}^{3+}(4f^{11})$ systems. This

Table 1
Hamiltonian parameters (in cm^{-1}) obtained from crystal-field (CF) and δ-function correlation-crystal-field (CCF) analyses of $\mathrm{LaCl_3{:}Pr^{3+}}$ and $\mathrm{GdCl_3{:}Pr^{3+}}$ energy-level data

Parameter	$\mathrm{LaCl_3{:}Pr^{3+}}$		$\mathrm{GdCl_3{:}Pr^{3+}}$	
	CF	CCF	CF	CCF
E_{avg}	9931(1)	9931(1)	9915(4)	9913(4)
F^2	68 440(12)	68 441(10)	68 136(46)	68 173(44)
F^4	50 183(37)	50 170(31)	50 099(158)	50 077(140)
F^6	32 973(19)	32 980(17)	32 918(85)	32 933(75)
α	22.8(0.1)	22.8(0.1)	22.6(0.3)	22.7(0.3)
β	−681(8)	−680(7)	−665(18)	−675(16)
δ	1453(7)	1453(6)	[1453]	[1453]
ξ	749(1)	749(1)	750(3)	750(2)
M^0	1.81(0.15)	1.81(0.12)	2.02(0.42)	1.98(0.37)
P^2	235(26)	237(22)	[237]	[237]
B^2_0	104(6)	97(6)	111(11)	109(10)
B^4_0	−337(14)	−343(13)	−438(34)	−399(34)
B^6_0	−653(20)	−663(17)	−781(62)	−781(55)
B^6_6	447(13)	445(11)	447(29)	483(25)
D^2_0	—	−0.9(1.3)	—	−2.8(1.9)
D^4_0	—	4.6(1.0)	—	6.0(2.2)
N[a]	60	60	35	35
σ[b]	6.8	5.7	8.6	7.3
$\sigma(^1D_2)$	17.2	6.6	18.0	7.6

[a] Number of experimental energy levels included in the data fits.
[b] Root-mean-square deviation between calculated and observed energy-level data (in cm^{-1}).

Table 2
Hamiltonian parameters (in cm^{-1}) obtained from crystal-field (CF) and δ-function correlation-crystal-field (CCF) analyses of hexachloride(elpasolite):Pr^{3+} energy-level data

Parameter	$\mathrm{Cs_2NaPrCl_6}$		$\mathrm{Cs_2NaYCl_6{:}Pr^{3+}}$	
	CF	CCF	CF	CCF
E_{avg}	10 201(3)	10 201(3)	10 198(4)	10 199(3)
F^2	67 809(46)	67 858(43)	67 750(53)	67 789(49)
F^4	50 375(117)	50 377(101)	50 126(162)	50 147(143)
F^6	32 979(73)	33 005(64)	32 879(84)	32 912(76)
α	23.5(0.4)	23.8(0.4)	24.3(0.5)	24.6(0.5)
β	−636(19)	−656(18)	−632(21)	−651(20)
δ	[1452]	[1452]	[1452]	[1452]
ξ	748(2)	748(1)	747(2)	746(2)
M^0	[1.81]	[1.81]	[1.81]	[1.81]
P^2	129(46)	143(41)	157(48)	175(44)
B^4_0	2178(33)	2173(28)	2279(35)	2270(30)
B^6_0	263(20)	254(18)	293(15)	285(14)
D^4_0	—	−6.1(2.3)	—	−5.8(2.4)
N[a]	27	27	27	27
σ[b]	9.8	8.2	10.1	8.6
$\sigma(^1D_2)$	14.6	1.9	14.0	1.3

[a] Number of experimental energy levels included in the data fits.
[b] Root-mean-square deviation between calculated and observed energy-level data (in cm^{-1}).

Table 3
Hamiltonian parameters (in cm^{-1}) obtained from crystal-field (CF) and δ-function correlation-crystal-field (CCF) analyses of $\mathrm{LiYF_4{:}Pr^{3+}}$ and $\mathrm{LiBiF_4{:}Pr^{3+}}$ energy-level data

Parameter	$\mathrm{LiYF_4{:}Pr^{3+}}$		$\mathrm{LiBiF_4{:}Pr^{3+}}$	
	CF	CCF	CF	CCF
E_{avg}	10 203(5)	10 204(3)	10 196(7)	10 196(5)
F^2	68 979(57)	69 025(41)	69 035(73)	69 097(57)
F^4	50 619(154)	50 580(109)	50 716(231)	50 685(173)
F^6	33 276(127)	33 326(91)	33 344(164)	33 387(125)
α	[23.0]	[23.0]	[23.0]	[23.0]
β	−637(30)	−649(21)	−641(40)	−647(30)
δ	[1371]	[1371]	[1371]	[1371]
ξ	750(3)	750(2)	752(4)	753(3)
M^0	[2.00]	[2.00]	[2.00]	[2.00]
P^2	220(96)	215(68)	156(120)	165(90)
B^2_0	433(41)	542(48)	369(56)	561(82)
B^4_0	−1068(72)	−1093(51)	−862(107)	−879(80)
B^4_4	1319(44)	1327(32)	1367(68)	1286(55)
B^6_0	−67(77)	−45(55)	−37(136)	−80(108)
B^6_4	1187(60)	1165(42)	1040(89)	1085(61)
D^2_0	—	−15.9(5.5)	—	−21.0(8.1)
D^4_0[a]	—	8.8(1.6)	—	8.2(1.9)
N[b]	46	46	36	36
σ[c]	22.6	15.5	25.7	18.4
$\sigma(^1D_2)$	40.6	10.8	30.8	7.9

[a] D^4_4/D^4_0 ratio held fixed according to B^4_4/B^4_0 ratio.
[b] Number of experimental energy levels included in the data fits.
[c] Root-mean-square deviation between calculated and observed energy-level data (in cm^{-1}).

Table 4
Hamiltonian parameters (in cm^{-1}) obtained from crystal-field (CF) and δ-function correlation-crystal-field (CCF) analyses of $CsCdBr_3$:Pr^{3+} energy-level data

Parameter	CF	CCF
E_{avg}	10 051(8)	10 050(8)
F^2	67 487(60)	67 477(57)
F^4	49 587(260)	49 581(249)
F^6	32 671(158)	32 689(153)
α	23.8(0.6)	23.6(0.6)
β	[−682.98]	[−682.98]
δ	[1422]	[1422]
ξ	744(3)	744(3)
M^0	1.4(0.5)	1.5(0.5)
P^2	[200]	[200]
B^2_0	−158(30)	−203(43)
B^4_0	−1192(62)	−1115(71)
B^4_3	1367(34)	1393(33)
B^6_0	362(73)	381(73)
B^6_3	271(45)	266(43)
B^6_6	39(53)	2(53)
D^2_0	—	9.4(6.7)
D^{4a}_0	—	2.7(1.5)
N^b	40	40
σ^c	11.1	10.1
$\sigma(^1D_2)$	10.6	1.3

[a] D^4_3/D^4_0 ratio held fixed according to B^4_3/B^4_0 ratio.
[b] Number of experimental energy levels included in the data fits.
[c] Root-mean-square deviation between calculated and observed energy-level data (in cm^{-1}).

model contains far fewer independent parameters than must be dealt with in applications of the general CCF model, which has crucially important advantages in dealing with systems for which only relatively small data sets are available. It is also especially advantageous in dealing with crystal-field splitting anomalies confined to just a few multiplet manifolds of a given system.

3. Results and discussion

Tables 1–4 compare the complete energy-level Hamiltonian parametrization, both without and with inclusion of the CCF δ-function parameters $D^{(2)}$ and $D^{(4)}$, for each of the seven Pr^{3+} systems examined. Table 1 compares parameter values for $LaCl_3$:Pr^{3+} and $GdCl_3$:Pr^{3+}, Table 2 compares parameter values for $Cs_2NaPrCl_6$ and Cs_2NaYCl_6:Pr^{3+}, Table 3 compares parameter values for $LiYF_4$:Pr^{3+} and $LiBiF_4$:Pr^{3+}, and Table 4 compares parameter values for $CsCdBr_3$:Pr^{3+}. Rank-2 crystal-field terms are forbidden in the cubic elpasolite structure, thus only a single CCF δ-function term $D^{(4)}$ is included in Table 2. In each table, statistical parameter uncertainties are given in parentheses after each parameter value. Experimental data were taken from Ref. [17] for $LaCl_3$:Pr^{3+}, from Ref. [18] for $GdCl_3$:Pr^{3+}, from

Table 5
Experimentally observed and calculated crystal-field energy levels (in cm^{-1}) for the $^1D_2$ multiplet in each host system

System	Γ	Expt.	CF calc.	Δ	CCF Calc.	Δ
$LaCl_3$:Pr^{3+}	A'	16 630.5	16 643.8	−13.3	16 632.3	−3.4
	E'	16 730.9	16 741.2	−10.3	16 737.4	−6.5
	E''	16 780.5	16 756.0	24.5	16 771.2	9.3
	σ			*17.2*		*6.6*
$GdCl_3$:Pr^{3+}	A'	16 565	16 579	−14	16 572	−7
	E'	16 683	16 694	−11	16 685	−2
	E''	16 747	16 721	26	16 736	11
	σ			*18*		*8*
$Cs_2NaPrCl_6$	T_2	16 670	16 684	−14	16 668	2
	E	17 253	17 238	15	17 255	−2
	σ			*15*		*2*
Cs_2NaYCl_6:Pr^{3+}	T_2	16 647	16 661	−14	16 646	1
	E	17 255	17 241	14	17 256	−1
	σ			*14*		*1*
$LiYF_4$:Pr^{3+}	B	16 746	16 815	−69	16 744	2
	A	16 813	16 798	15	16 798	15
	E	17 092	17 064	28	17 107	−15
	B	17 408	17 380	28	17 411	−3
	σ			*41*		*11*
$LiBiF_4$:Pr^{3+}	B	16 744	16 795	−51	16 735	9
	A	16 847	16 839	8	16 840	7
	E	17 086	17 054	32	17 091	−5
	B	17 391	17 379	12	17 401	−10
	σ			*31*		*8*
$CsCdBr_3$:Pr^{3+}	E	16 540	16 540	0	16 539	1
	A_1	16 570	16 583	−13	16 569	1
	E	17 011	16 998	13	17 013	−2
	σ			*11*		*1*

Ref. [19] for $Cs_2NaPrCl_6$ and Cs_2NaYCl_6:Pr^{3+}, from Ref. [20] for $LiYF_4$:Pr^{3+} and $LiBiF_4$:Pr^{3+}, and from Ref. [21] for $CsCdBr_3$:Pr^{3+}.

As can be seen from the parameter values given in Tables 1–4, inclusion of the CCF δ-function parameters has no significant effect upon the standard atomic and crystal-field parameter values. Since the CCF δ-function only considers correlation effects from two electrons in the same orbital (with opposite spins), the $D^{(k)}$ parameters selectively affect the singlet multiplets $^1D_2$, $^1G_4$, and $^1I_6$, leaving calculated energy levels for the triplet multiplet manifolds ^3H_J, ^3F_J, and ^3P_J unchanged.

Root-mean-square deviations between calculated and observed energy-levels, given in the last two rows of Tables 1–4, show a small but significant improvement in the overall fitting of all experimentally determined levels, with a pronounced improvement in the fitting of the $^1D_2$ multiplet manifold. Table 5 presents details of the fittings to the $^1D_2$ multiplet manifold for each of the seven systems examined. As can be seen from this table, inclusion of the CCF δ-function parameters well explains the anomalous splittings of this multiplet for each system.

4. Conclusion

Incorporation of CCF δ-function interaction terms into $Pr^{3+}(4f^2)$ energy-level modeling calculations is effective in resolving the major discrepancies between observed and calculated crystal-field splittings in the infamous $^1D_2$ multiplet manifold. Moreover, we have shown that the augmented model Hamiltonian used in these calculations requires at most two more interaction parameters beyond those included in the ‘standard’ model Hamiltonian. This work expands upon our earlier preliminary analysis [25], and represents the first systematic application of the CCF δ-function model in analyses of crystal-field energy-level data. It is not clear whether the interactions represented in this model should be considered more important than those represented in the crystal-field-induced configuration–interaction model employed in recent work by Faucher and Moune [11], or whether there may be a formalistic relationship between these two different calculation methods. However, as was noted earlier, systematic applications of the latter model pose major computational problems, due in large part to the necessity of dealing explicitly with excited configurations, the detailed properties of which are generally ill-characterized.

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