THE CALCULATION METHOD FOR SPHERICAL OPERATORS IN MALKIN'S MODEL

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Abstract: *The model was introduced by Malkin (ECM) to describe the behavior of rare earth metals (RE) and transition metals (TM) used as an impurity ion crystal field of ligands belonging to the crystal (host matrix).The calculation is quite easy for those who apply irreducible tensor operators MAPLE programming introduced by Malkin.*

Keywords: Malkin's model, load sharing model, ECM, single particle operators.

Introduction: For this model crystal field Hamiltonian (Hamiltonian of interaction between ligand field and impurity ions) is calculated according to the relation: $H_{cr} = \sum_{p=0}^{2l} \sum_{k=-p}^{p} B_p^k O_p^k$ **(1.1)**

where B_p^k are crystal field parameters of the ligand and are calculated as a sum of two contributions:

$$B_p^k = B_{p,q}^k + B_{p,s}^k \quad \textbf{(1.2)}$$

$$B_{p,q}^k = -K_p^k e^2 \left\langle r^p \right\rangle \sum_i q_i \frac{V_p^k(\theta_i, \varphi_i)}{R_i^{p+1}} \quad \textbf{(1.3)}$$

$$B_{p,s}^k = K_p^k e^2 \frac{2(2p+1)}{5} \sum_i \left(G_s S_s(i)^2 + G_\sigma S_\sigma(i)^2 + \gamma_p G_\pi S_\pi(i)^2 \right) \frac{V_p^k(\theta_i, \varphi_i)}{R_i^{p+1}} \quad \textbf{(1.4)}$$

Irreducible tensor operators O_p^k introduced by Malkin acting on angular parts of wave functions ψ and are single particle operators.

$$O_p{}^k = \frac{1}{a_{pk}} Z_p^k, \quad \textbf{(1.5)}$$

where a_{pk} sunt factori numerici tabelați, and Z_p^K is calculated using the harmonic formula:

$$Z_p^K = \begin{cases} C_p^{-k} + (-1)^k C_p^k, k \rangle 0 \\ C_p^k, k = 0 \\ -i\left(C_p^{-k} - (-1)^k C_p^k\right), k \langle 0 \end{cases} \quad \textbf{(1.6)}$$

Irreducible tensor operators O_p^k are calculated on the basis of spherical single particle operators play by the following relation:

$$C_q^{(k)} = \sqrt{\frac{4\pi}{2k+1}} Y_p^k \quad \textbf{(1.7)}$$

where Y_p^k spherical harmonics are calculated by Malkin's model with its annexes.

Analysis model: Calculation of spherical harmonic functions

> # Calculation of the table of coefficients angular coordinates (alpha,beta,gamma1) I took a[i] vector line format i no Ri(last item on the line i table) then put b[i] then transposed alpha[i]:=a[i].E1/(a[i].b[i]);beta[i]:=a[i].E2/(a[i].b[i]); gamma1[i]:=a[i].E3/(a[i].b[i]);where E1:=<1,0,0>:E2:=<0,1,0>:E3:=<0,0,1>: I copied the line copies i table and put the program. I made 45 copies linii.merge repede.se line i is put in front a[i]:=< line elements i cu | between components >: then put b[i]:=< line elements i with , between components >: and still put in the table below. for n put how many lines are. When working with the other program is adding to S:=sum(F(i),i=1..n);

> with(LinearAlgebra):

> E1:=<1,0,0>:E2:=<0,1,0>:E3:=<0,0,1>:

> n:=45;

>a:=array(0..n):b:=array(0..n):x:=array(0..n):x:=array(0..n):x:=array(0..n): a[1]:=<-1.9985e-05|-2.0507|1.9985e-05>:b[1]:=<-1.9985e-05,-2.0507,1.9985e-05>: a[2]:=<-1.9985e-05|2.9913e-05|-2.0507>:b[2]:=<-1.9985e-05,2.9913e-05,-2.0507>: a[3]:=<2.0507|2.9913e-05|1.9985e-05>:b[3]:=<2.0507,2.9913e-05,1.9985e-05>: a[4]:=<-1.9985e-05|2.0508|1.9985e-05>:b[4]:=<-1.9985e-05,2.0508,1.9985e-05 >: a[5]:=<-2.0508|2.9913e-05|1.9985e-05>:b[5]:=<-2.0508,2.9913e-05,1.9985e-05>: a[6]:=<-1.9985e-05|2.9913e-05|2.0508>:b[6]:=<-1.9985e-05,2.9913e-05,2.0508>: a[7]:=<2.0507|-2.0507|1.9985e-05>:b[7]:=<2.0507,-2.0507,1.9985e-05>: a[8]:=<-1.9985e-05|-2.0507|-2.0507>:b[8]:=<-1.9985e-05,-2.0507,-2.0507>:

a[9]:=<2.0507|2.9913e-05|-2.0507>:b[9]:=<2.0507,2.9913e-05,-2.0507>:

a[10]:=<-2.0508|2.0508|1.9985e-05>:b[10]:=<-2.0508,2.0508,1.9985e-05>:

a[11]:=<-1.9985e-05|2.0508|2.0508>:b[11]:=<-1.9985e-05,2.0508,2.0508>: a[12]:=<-2.0508|2.9913e-05|2.0508>:b[12]:=<-2.0508,2.9913e-05,2.0508>:

a[13]:=<-1.0254|-3.0761|1.0254>:b[13]:=<-1.0254,-3.0761,1.0254>:

a[14]:=<-1.0254|1.0254|-3.0761>:b[14]:=<-1.0254,1.0254,-3.0761>:

a[15]:=<3.0761|1.0254|1.0254>:b[15]:=<3.0761,1.0254,1.0254>:

Results and discussion:

V_p^k - depend on the spherical coordinates of the crystal lattice doped with impurity ions.

V_p^k - are polynomials that depend spherical spherical coordinates θ_i si φ_i of ligands.

According to Cartesian coordinates (x, y, z) and angular (α, β, γ) we have the following relations: $\alpha = x/r, \beta = y/r, \gamma = z/r$

In the calculation of V_p^k, we have: $\alpha = \frac{x}{r}$, $\beta = \frac{y}{r}$, $\gamma = \frac{z}{r}$, where $r = \sqrt{x^2 + y^2 + z^2}$

Spherical harmonics are defined by the **(1.8),** with $V \rightarrow Y$

$$Y_l^m = (-1)^q \Xi_l^m \cdot (2\pi)^{-1/2} \cdot e^{im\varphi} \qquad \textbf{(1.8)}$$

Associated polynomials are defined by functions Ξ_l^m:

$$\Xi_0^0 = (1/2)^{1/2}$$
$$\Xi_1^0 = (3/2)^{1/2} \cdot \cos\theta$$
$$\Xi_1^1 = (3/4)^{1/2} \cdot \sin\theta$$
$$\Xi_2^0 = (5/8)^{1/2} \cdot (3\cos^2\theta - 1)$$
$$\Xi_2^1 = (15/4)^{1/2} \cdot \sin\theta\cos\theta$$
$$\Xi_2^2 = (15/16)^{1/2} \cdot \sin^2\theta$$
$$\Xi_3^0 = (7/8)^{1/2} \cdot (5\cos^3\theta - 3\cos\theta)$$
$$\Xi_3^1 = (21/32)^{1/2} \cdot \sin\theta \cdot (5\cos^2\theta - 1)$$
$$\Xi_3^2 = (105/16)^{1/2} \cdot \sin^2\theta\cos\theta$$
$$\Xi_3^3 = (35/32)^{1/2} \cdot \sin^3\theta$$
$$\Xi_4^0 = (9/128)^{1/2} \cdot (35\cos^4\theta - 30\cos^2\theta + 3)$$
$$\Xi_4^1 = (45/32)^{1/2} \cdot \sin\theta \cdot (7\cos^3\theta - 3\cos\theta)$$
$$\Xi_4^2 = (45/64)^{1/2} \cdot \sin^2\theta \cdot (7\cos^2\theta - 1)$$
$$\Xi_4^3 = (315/32)^{1/2} \cdot \sin^3\theta \cdot \cos\theta$$
$$\Xi_4^4 = (315/256)^{1/2} \cdot \sin^4\theta$$

Conclusions:

Spherical tensor operators were refined using the computer program MAPLE.

Experimental and theoretical energy levels are calculated based on crystal field parameters determined and the spherical tensor operators and investigated the energy levels are well described by crystal field.

References:

1. Călin N. Avram – Vibronic laser $LiCaAlF_6$:$Cr^{3+,}$ Publishing Mirton, Timisoara 2004.

2. Nicolae M. Avram – Energy levels of ions in crystals, Publishing Mirton, Timisoara 2001.

3. Gîrdu Constantin Cristinel - Report no. 3, West University of Timisoara.