Determination of tetragonal crystalline electric field parameters  
for Yb3+ and Ce3+ ions from experimental *g‑*factors values  
and energy levels of Kramers doublets  
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The tetragonal crystalline electric field parameters for Yb3+ and Ce3+ ions are expressed via ground multiplet exited doublets energies and parameters defining doublets’ wave functions. The crystalline electric field parameters for Yb3+ ion in YbRh2Si2, YbIr2Si2 and KMgF3 crystals extracted from excited state doublets energies and *g*-factors of ground state doublet are compared with parameters determined in other works. {***No more than 200 words. Use the MRSej style of paragraph named “\_MRSej\_Abstract”*** }

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1. Introduction {Use the MRSej style of paragraph named “*\_MRSej\_Section*” }

Our work was initially stimulated by investigation of heavy-fermion Kondo lattice compounds. Very peculiar magnetic, thermal and transport properties of 4*f*‑electron based heavy-fermion systems are determined by the interplay of the strong repulsion of 4*f‑*electrons on the rare-earth ion sites, their hybridization with wide-band conduction electrons and an influence of the crystalline electric field. {***For first paragraph* *use the MRSej style of paragraph named “\_MRSej\_TextNonIndent”*** }

In this paper we present the detailed calculation of CEF parameters from energies of ground multiplet exited Kramers doublets and *g*-factors of ground state Kramers doublet. {***Use the basic MRSej style of paragraph named “\_MRSe\_Text\_Main”***

2. Diagram of Yb3+ *g*‑factors

A free Yb3+ ion has a 4*f*13 configuration with one term 2*F*. The spin-orbit interaction splits the 2*F* term into two multiplets: 2*F*7/2 with *J* = 7/2 and 2*F*5/2 with *J* = 5/2, where *J* is value of the total momentum **J** = (*Jx*, *Jy*, *Jz*). Multiplets are separated by about 1 eV [4]. The Hamiltonian of the Yb3+ ion interaction with the tetragonal CEF could be written via equivalent operators  [4]: {***Below we use the MRSej style of paragraph named “\_MRSej\_Eq”***}

{***One tab before***} , {***One tab after*}** (1)

where  are the CEF parameters, *α* = 2/63, *β* = −2/1155, *γ* = 4/27027 [4]. {***After equations we use*** ***“\_MRSej\_TextNonIndent” or “\_MRSe\_Text\_Main”***}

As follows from the group theory, the two-valued irreducible representation *D*7/2 of rotation group contains two two-dimensional irreducible representations of the double tetragonal group [4]. ……………………………………..

The former results correspond to bases |5/2〉, |−3/2〉 and |−5/2〉, |3/2〉, the latter corresponding to bases |7/2〉, |−1/2〉 and |−7/2〉, |1/2〉. It is convenient to introduce parameters *C*, *A* and *D*:

, . (2)

Since matrices (2) are diagonal in the bases of their eigenvectors we can find the relations between our angular parameters and CEF parameters: tan *φ*7 = *C*3/*C*, tan *φ*6 = *A*3/*A*, it is enough to take −*π*/2 ≤ *φ*7, *φ*6 ≤ *π*/2.

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| **Table 1*.*** Energies, wave functions and *g*‑factors of  Yb3+ ion in tetragonal crystalline electric field. {***“\_MRSej\_table\_caption"*** }   |  |  | | --- | --- | |  | {***“\_MRSej\_tableIn”***} | |  |  | | …………… ………………. | ………………… ………………… | |

EPR spectra of Yb3+ ions {**“\_MRSej\_SubSection”**}

The Zeeman energy *gJ*B**HJ** in the basis |↑〉, |↓〉 of each doublet could be represented by matrix

, (3)

|  |
| --- |
| {**Figures and tables are inserted into tables**}  Figure **1**. The diagram of *g*‑factors of Yb3+ ion in tetragonal crystalline electric field and experimental *g*‑points taken from literature (tab. 2). {***“\_MRSej\_figure\_caption”*** } |

where **H** is the magnetic field, **S** is the effective spin operator with S = 1/2, *μ*B is the Bohr magneton, *g*|| and *g*⊥ are *g*‑factors when the field is applied parallel and perpendicular to the tetragonal *z*‑axis, respectively (tab. 1) The field is applied parallel and perpendicular to the tetragonal *z*‑axis, respectively.

EPR spectra in cubic symmetry case

In the case of cubic symmetry , , , , , . In accordance with expansion  [4] the doublets  and 

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Table 2.** Experimental *g*‑factors of Yb3+ ion in tetragonal crystalline electric field given in figure 1.   |  |  |  | | --- | --- | --- | |  | YbRh2Si2 [1] | YbIr2Si2 [2] | |  | 0.17(7) | 0.85(1) | |  | 3.561(6) | 3.357(5) | |

………….

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Using the least squares method the experimental values of *g*‑factors (tab. 2) and experimental energy of whole 2*F* term levels have been taken into account. Obtained CEF parameters satisfy the experimental energy scheme of 2*F* term very well, but are reproduced by our expressions (9) only approximately (tab. 5).

4. Calculation of CEF parameters for Yb3+ ion. Comparison with another papers

Let us calculate the CEF parameters for the given exited state doublets energies Δ1 < Δ2 < Δ3. It follows from (3) that we find:

,

, , (9)

, ,

In paper [7] CEF parameters of Yb3+ ion in KMgF3 crystal have been found (tab. 5). Using the least squares method the experimental values of *g*‑factors (tab. 2) and experimental energy of whole 2*F* term levels have been taken into account. Obtained CEF parameters satisfy the experimental energy scheme of 2*F* term very well, but are reproduced by our expressions (9) only approximately (tab. 5).

|  |
| --- |
| Figure **2.** Temperature dependence of the strength of the potential *V* (see (6)), obtained from the simulation of C60 EPR spectra. |

In this case *g*|| and *g*⊥ are related by the equation , but as the admixture of excited 2*F*5/2 multiplet is small (*p*3 = 0.00551 [7]) we obtain previous relation *g*|| + 2*g*⊥ + 8 = 0. On the diagram (fig. 1) we marked experimental values of Yb3+ *g*‑factors in several crystals (see also tab. 2). This allows us to estimate the signs of *g*‑factors and to make assumptions about the ground state Kramers doublet on the basis of measured absolute values of *g*‑factors. For example, it is evident that the ground state doublet of Yb3+ ion in HfSiO4 is  and both parallel and perpendicular *g*‑factors have a negative sign. The ground state doublet of Yb3+ ion in KMgF3 is , the sign of *g*|| is positive, the sign of *g*⊥ is negative. In CaF2 crystal the tetragonal center of Yb3+ is in state  and the sign of *g*|| is positive but the sign of *g*⊥ can be both positive and negative.

4. Summary

For Yb3+ and Ce3+ ions all possible sets of tetragonal crystalline electric field parameters that satisfy the given experimental energy scheme of ground multiplet are defined.

The earlier published CEF parameters for Yb3+ ion in YbRh2Si2 and YbIr2Si2 crystals calculated with the use of least squares method could be obtained from our formulas (see tab. 5).

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