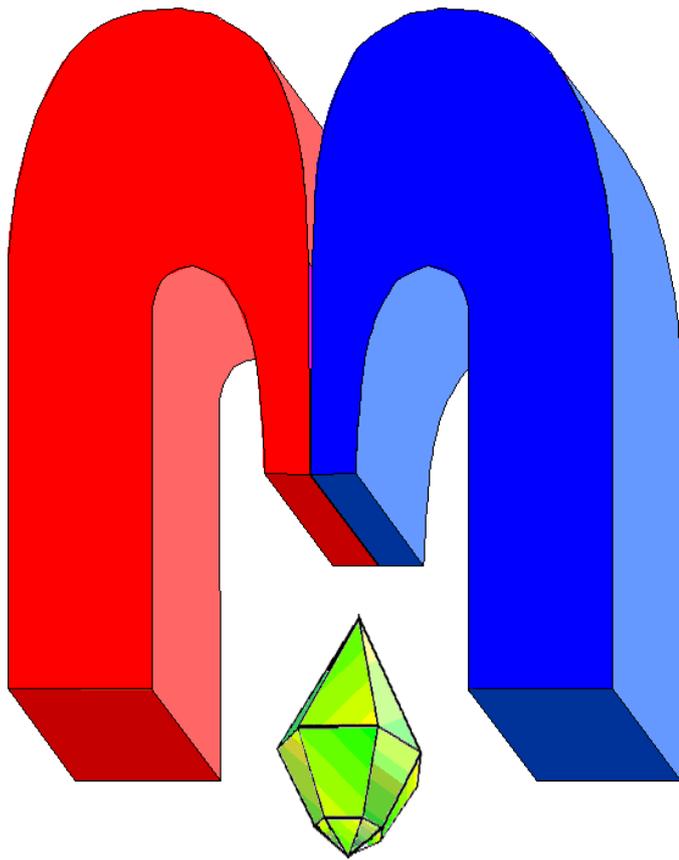


ISSN 2072-5981
doi: 10.26907/mrsej



***magnetic
Resonance
in Solids***

Electronic Journal

Volume 21

Issue 1

Paper No 19108

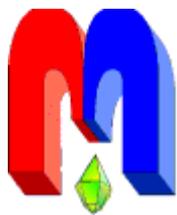
1-9 pages

2019

doi: 10.26907/mrsej-19108

<http://mrsej.kpfu.ru>

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Established and published by Kazan University
Endorsed by International Society of Magnetic Resonance (ISMAR)
Registered by Russian Federation Committee on Press (#015140),
August 2, 1996
First Issue appeared on July 25, 1997

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"Magnetic Resonance in Solids. Electronic Journal" (MRSej) is a peer-reviewed, all electronic journal, publishing articles which meet the highest standards of scientific quality in the field of basic research of a magnetic resonance in solids and related phenomena.

Indexed and abstracted by
Web of Science (ESCI, Clarivate Analytics, from 2015), Scopus (Elsevier, from 2012), RusIndexSC (eLibrary, from 2006), Google Scholar, DOAJ, ROAD, CyberLeninka (from 2006), SCImago Journal & Country Rank, etc.

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* In Kazan University the Electron Paramagnetic Resonance (EPR) was discovered by Zavoisky E.K. in 1944.

Tables of functions transforming according to the irreducible representations of crystal point cubic T and T_h groups

A.M. Leushin

Kazan Federal University, Kremlevskaya 18, Kazan 420008, Russia

E-mail: amleushin@gmail.com

(Received March 1, 2019; accepted March 5, 2019; published March 15, 2019)

The functions transforming according to the nonequivalent irreducible representations (IR) Γ'_2 , Γ'_3 and Γ'_6 , Γ'_7 have been found using the projection operators of the IR D_5 of the full rotation group on the subspaces of IR of T , T' and T_h , T'_h cubic groups. With allowance for the properties with respect to the operation of the time reversal sign, the functions are combined into representations Γ'_{23} and Γ'_{67} , respectively, of twice the larger dimension. Along with the functions transforming according to all other IRs Γ'_1 , Γ'_4 and Γ'_5 presented earlier, they will facilitate the consideration of various kinds of effects due to the energy level splitting of rare-earth ions in the crystal electric fields of T , and T_h group symmetry.

PACS: 31.15.xh, 71.70.Ch, 75.10.Dg, 76.30.Kg.

Keywords: crystal electrical fields, cubic T and T_h groups, function of irreducible representations, rare earth, EPR, inelastic neutron scattering spectra.

1. Introduction

Recently a large amount of work has been invested in the rare-earth (RE) compounds, in which the local point symmetry for RE ions is T_h . As examples of such compounds, it is possible to name the filled skutterudite compounds (FS) with the formula RT_4X_{12} or doped unfilled skutterudite, such as $CoSb_3$. In FS R is RE or actinide, T is a transition metal (Fe, Ru, Os) and X is a pnictogen (P, As, Sb) [1]. FS crystallize in the $LaFe_4P_{12}$ structure with space group $Im\bar{3}$ and local point symmetry T_h for the R ions. The R ions are located at the corners and body center of the cubic lattice, each of which is surrounded by a simple cube of 8 transition metal atoms at the 8c site and by a slightly deformed icosahedron of 12 pnictogen atoms at the 24g Wyckoff sites.

The notably mounting interests and efforts in studying the FS compounds, e.g. are motivated by the remarkable diversity of their electronic and magnetic ground states, including multipole ordering [2, 3], small gap insulators [4, 5], conventional superconductivity [6], unconventional superconductivity [7, 8], and magnetic ordering [9-13]. Despite the large differences in their physical properties, these compounds are governed by only a few parameters, including the interaction between the conduction and the 4f shell electrons (c-f coupling) and the effect of the crystal electric field (CEF) potential on the RE^{3+} 4f electrons [2-13]. Owing to their unique structure, a subtle modification on composition can result in a different CEF scheme and thus a completely different ground state.

Most of the important properties of other compounds as well, which include the RE ions, are also mainly determined by the behavior of the latter in CEF. The RE ions located in a crystal largely preserve their individuality, and the action of the crystal field leads to the splitting of their multiplet energy levels. The pattern of this splitting in transparent crystals is determined from the optical spectra of luminescence and absorption in the infrared and visible bands, while experiments to measure magnetic susceptibility, electron paramagnetic resonance (EPR) and inelastic magnetic neutron scattering are used in opaque crystals to establish this pattern. To identify the observed Stark structure of the energy levels, e.g., from EPR and optical spectra, or magnetic neutron scattering, it is necessary to theoretically calculate the positions of the CEF levels and the intensity of the assumed transitions, and then to compare them with the corresponding experimental values.

The necessary computations can be greatly simplified by using as the eigenfunctions of multiplets of RE ions not simply the functions $|JM_J\rangle$ of the total angular momentum J and its projection on the selected axis M_J , but their linear combinations, which implement the IR of the CEF point group. Such functions transforming according to all IR of all 32 crystal point groups (CPG) were found by author in 1968 [14]. In addition to the basis functions, tables [14] contain expansion formulas of all IR of the full rotation group (FRG) to $D_{17/2}$, inclusive, over IR of CPG (compatibility relations between the FRG and the CPG) making it possible to immediately answer the question to how many and what energy levels each multiplet of one or another RE ion in CEF of a given symmetry group is split. Many other CPG characteristics, such as expansion tables of IR direct products (multiplication tables), coupling coefficients, facilitating the calculations were presented in the book [15].

For example, it can be seen from the comparison of octahedron group O (432) and tetrahedron group T (23) that T is a subgroup of the O group and due to the absence in it of rotations by the angle of $\pi/2$ around the fourfold axes and the rotations by the angle of π around the twofold axes perpendicular to them the number of elements of the group T reduces from 24 to 12. This entails the changes in the number and properties of IR. If the octahedron group O has five representations: singlet Γ_1 (identity representation), singlet Γ_2 , doublet Γ_3 , triplet Γ_4 , triplet Γ_5 , and also the double group O' has three representations: doublet Γ_6 , doublet Γ_7 , and quartet Γ_8 (here and below for IR we use the Bethe notation system [16]), in the tetrahedron group T IRs are as follows: singlet Γ'_1 (identity representation), singlet Γ'_2 , singlet Γ'_3 , triplet Γ'_4 , and three representations of the double group T' : doublet Γ'_5 , doublet Γ'_6 and doublet Γ'_7 . The Γ'_2 and Γ'_3 singlets, and the Γ'_6 and Γ'_7 doublets have complex conjugate characters and are degenerate each other, respectively, by the time reversal symmetry. Therefore, the corresponding representations have always to be combined in physical applications: Γ'_2 and Γ'_3 singlets are considered together as the Γ'_{23} singlet-paired doublet and Γ'_6 and Γ'_7 doublets are considered as the Γ'_{67} doublet-paired quartet. In this respect, the splitting patterns of $(2J+1)$ multiples of RE ions by CEF of O group and T group symmetry are similar: the number of Stark-sublevels and the degeneracy of each sublevel are the same. However, due to the fact that IR Γ_2 of the O group at the transition to the T subgroup transforms into IR Γ'_1 of the T group, the identity IRs (invariants) of the T group in expansions of IR D_J of the FRG will be met oftener than IR Γ_1 (invariants) of the O group. In particular, at the expansion of the IR D_3 , the invariant $\sqrt{\frac{1}{2}}(Y_3^2 - Y_3^{-2})$ appears, and in the expansion of IR D_6 not one as in the O group but two invariants will be present [14]:

$$\left[\sqrt{\frac{1}{8}}Y_6^0 - \sqrt{\frac{7}{16}}(Y_6^4 + Y_6^{-4}) \right] \quad \text{and} \quad \left[\sqrt{\frac{11}{32}}(Y_6^2 + Y_6^{-2}) - \sqrt{\frac{5}{32}}(Y_6^6 + Y_6^{-6}) \right].$$

The eigenvalues and eigenfunctions of RE ions in CEF of T group will differ from the corresponding quantities in the CEF of the O group, because now they will have to be found from the diagonalization of higher order matrices, in which the states of the same IR will be coupled. For example, two different IR Γ_4 and Γ_5 of O group become the same representation Γ'_4 of the T group, analogously, two different IR Γ_6 and Γ_7 of the O' group transform into one representation Γ'_5 of the T' group. The transformed eigenfunctions, naturally, result in the change of the selection rules and intensities of the possible transitions.

All these considerations were known to researchers involved in EPR and optical spectroscopy of crystals containing RE ions, however, they remained unclaimed, since there were no compounds in the field of view of physicists, in which RE ions would be in positions with CEF with the symmetry of either T or T_h groups. The situation changed after in 2001, Takegara et al [17] indicated two types of compounds, in which RE ions are subjected to CEF with symmetry of the group T_h . One of the compounds is the filled skutterudite with the general formula RT_4X_{12} , and the second compound is RPd_3S_4 crystallizing in the structure of the $NaPt_3O_4$ type. The authors [17] emphasized the presence of

the additional six-order term in the Hamiltonian of the interaction of RE ion with CEF having the T_h group symmetry

$$B_6 \left[C_{6-2} + C_{62} - \sqrt{\frac{5}{11}}(C_{6-6} + C_{66}) \right] \quad (C_{kq} \text{ is the operator of the spherical function}),$$

which is absent in CEF of O , T_d and O_h groups. Their work stimulated the emergence of a large number of studies, in which the value of the B_6 parameter was determined and the effect of the additional term on magnetic scattering of neutrons [18, 19], EPR spectra [20, 21], and other properties of the considered compounds [22] was analyzed.

To facilitate the necessary computations, it is advisable to use the functions of multiplets of RE ions, published in [14]. However, in the tables with functions that are transformed according to the representations Γ'_{23} and Γ'_{67} of the cubic T and T_h groups, the transformations were carried out, which led to the loss of the properties of the rows of the initial IR Γ'_2 and Γ'_3 singlets and Γ'_6 and Γ'_7 doublets. The fact is that in physical applications of the theory of some groups, the complex conjugate nonequivalent IR they have, due to the properties of the functions transformed according to them, with respect to the time reversal operation, should be combined into representations of twice the dimension [23]. The cubic T and T_h groups have such IR Γ'_2 and Γ'_3 singlets and Γ'_6 and Γ'_7 doublets. The author [14] performed the necessary unifications and in addition, combined the basis functions in the spaces of the united representations so as to obtain their simpler expressions. As a result, new functions have lost their properties of IR of T and T_h groups and transformed essentially into the basis functions of IR Γ_3 and Γ_8 of O and O' groups, respectively.

The purpose of this work is to present tables of correct functions that are transformed by representations Γ'_{23} and Γ'_{67} of T and T_h groups, in which the functions IR Γ'_2 and Γ'_3 and IR Γ'_6 and Γ'_7 would be simply united into representations of twice the larger dimension without any additional transformations of the basis functions.

In the proposed tables, we will follow the same system of notations as was used in [14]. Namely, each function $\Psi_{\Gamma_{\alpha j}}$ transforming as the j -th component of some IR Γ_{α} is a linear combination of the form $\Psi_{\Gamma_{\alpha j}} = \sum_m a_{\alpha j}^m \Psi_{S_m}$, where the functions Ψ_{S_m} , perform IR D_S of the rotation group and are transformed as the eigenfunctions of the operator of angular momentum. The subscript S corresponds to the value of the angular momentum and m its projection on the selected axis. To reduce the size of the tables, we present not the coefficients themselves, $a_{\alpha j}^m$, but the squares of their absolute values $|a_{\alpha j}^m|^2 = C_m$, which are simply denoted as C_m , omitting the subscripts of the representation and its components, because they are fixed on the left of each function. If the coefficients $a_{\alpha j}^m$ are imaginary, the asterisk is put on the top left at the quantity C_m . Its presence requires the multiplication by the imaginary unity "i" of the coefficient $a_{\alpha j}^m$, which is obtained after extracting the positive square root of the corresponding value C_m . The cases when the square roots should be taken with a negative sign are indicated by asterisks from the top left of the corresponding numerical C_m values. Tables show only the nonzero C_m values. If in the expansion of any IR D_S of the rotation group the same IR of T and T_h groups are met several times, the functions of different similar representations are numbered with 1, 2, 3, which are put on the top left of the number denoting the representation. The transformation properties of the found functions are fixed by IR of the T group, the number of which is written in the second column. The component of the representation is indicated following it. For the sake of abbreviation, representations are simply indicated by their number α . For the same reasons, the component of the representation is simply denoted by the corresponding number 1, 2. The number of IR of the O group, at the expansion of which these representations of its T subgroup appear, is given in the first column.

2. Tables of functions of T group

In the Tables below, the basis functions for the T group can be objects of any nature with respect to spatial inversion. For the T_h group, in the case of even objects with respect to spatial inversion, add the index "g" and the index "u" for odd objects to the notations of all IRs.

$S = 3/2$		$D_{3/2} = \Gamma'_{67}$						
8	$67'$	$6'$	1	$C_{-1/2} = 1/2$	$*C_{3/2} = *1/2$			
			2	$C_{1/2} = 1/2$	$*C_{-3/2} = *1/2$			
		$7'$	1	$C_{-1/2} = 1/2$	$*C_{3/2} = 1/2$			
			2	$C_{1/2} = 1/2$	$*C_{-3/2} = 1/2$			
$S = 2$		$D_2 = \Gamma'_{23} + \Gamma'_4$						
3	$23'$	$2'$	1	$C_0 = 1/2$	$*C_2 = 1/4$	$*C_{-2} = 1/4$		
		$3'$	1	$C_0 = 1/2$	$*C_2 = *1/4$	$*C_{-2} = *1/4$		
$S = 5/2$		$D_{5/2} = \Gamma'_5 + \Gamma'_{67}$						
8	$67'$	$6'$	1	$C_{-1/2} = *1/2$	$*C_{3/2} = 1/12$	$*C_{-5/2} = 5/12$		
			2	$C_{1/2} = 1/2$	$*C_{-3/2} = *1/12$	$*C_{5/2} = *5/12$		
		$7'$	1	$C_{-1/2} = *1/2$	$*C_{3/2} = *1/12$	$*C_{-5/2} = *5/12$		
			2	$C_{1/2} = 1/2$	$*C_{-3/2} = 1/12$	$*C_{5/2} = 5/12$		
$S = 3$		$D_3 = \Gamma'_1 + 2\Gamma'_4$						
2		$1'$	1	$C_2 = 1/2$	$C_{-2} = *1/2$			
$S = 7/2$		$D_{7/2} = 2\Gamma'_5 + \Gamma'_{67}$						
8	$67'$	$6'$	1	$C_{-1/2} = *5/24$	$C_{7/2} = 7/24$	$*C_{3/2} = *3/8$	$*C_{-5/2} = *1/8$	
			2	$C_{1/2} = *5/24$	$C_{-7/2} = 7/24$	$*C_{-3/2} = *3/8$	$*C_{5/2} = *1/8$	
		$7'$	1	$C_{-1/2} = *5/24$	$C_{7/2} = 7/24$	$*C_{3/2} = 3/8$	$*C_{-5/2} = 1/8$	
			2	$C_{1/2} = *5/24$	$C_{-7/2} = 7/24$	$*C_{-3/2} = 3/8$	$*C_{5/2} = 1/8$	
$S = 4$		$D_4 = \Gamma'_1 + \Gamma'_{23} + 2\Gamma'_4$						
3	$23'$	$2'$	1	$C_4 = C_{-4} = 7/48$	$C_0 = *5/24$	$*C_2 = 1/4$	$*C_{-2} = 1/4$	
		$3'$	1	$C_4 = C_{-4} = 7/48$	$C_0 = *5/24$	$*C_2 = *1/4$	$*C_{-2} = *1/4$	
$S = 9/2$		$D_{9/2} = \Gamma'_5 + 2\Gamma'_{67}$						
18	$^167'$	$^16'$	1	$C_{7/2} = *7/32$	$C_{-9/2} = 7/32$	$C_{-1/2} = *1/16$	$*C_{3/2} = *1/2$	
			2	$C_{9/2} = *7/32$	$C_{-7/2} = 7/32$	$C_{1/2} = 1/16$	$*C_{-3/2} = 1/2$	
		$^17'$	1	$C_{7/2} = *7/32$	$C_{-9/2} = 7/32$	$C_{-1/2} = *1/16$	$*C_{3/2} = 1/2$	
			2	$C_{9/2} = *7/32$	$C_{-7/2} = 7/32$	$C_{1/2} = 1/16$	$*C_{-3/2} = *1/2$	

2_8	${}^2_6 7'$	${}^2_6'$	1	$C_{7/2} = 25/96$	$C_{-1/2} = *7/48$	$C_{-9/2} = 3/32$	$*C_{-5/2} = *1/2$
			2	$C_{9/2} = *3/32$	$C_{1/2} = 7/48$	$C_{-7/2} = *25/96$	$*C_{5/2} = 1/2$
	${}^2_7'$		1	$C_{7/2} = 25/96$	$C_{-1/2} = *7/48$	$C_{-9/2} = 3/32$	$*C_{-5/2} = 1/2$
			2	$C_{9/2} = *3/32$	$C_{1/2} = 7/48$	$C_{-7/2} = *25/96$	$*C_{5/2} = *1/2$

$$S = 5 \quad D_5 = \Gamma'_{23} + 3\Gamma'_4$$

3	$23'$	$2'$	1	$C_4 = 1/4$	$C_{-4} = *1/4$	$*C_2 = *1/4$	$*C_{-2} = 1/4$
		$3'$	1	$C_4 = 1/4$	$C_{-4} = *1/4$	$*C_2 = 1/4$	$*C_{-2} = *1/4$

$$S = 11/2 \quad D_{11/2} = 2\Gamma'_5 + 2\Gamma'_{67}$$

1_8	${}^1_6 7'$	${}^1_6'$	1	$C_{7/2} = *1/12$	$C_{-9/2} = 5/12$	$*C_{3/2} = *1/6$	$*C_{-5/2} = 1/3$
			2	$C_{9/2} = 5/12$	$C_{-7/2} = *1/12$	$*C_{5/2} = 1/3$	$*C_{-3/2} = *1/6$
	${}^1_7'$		1	$C_{7/2} = *1/12$	$C_{-9/2} = 5/12$	$*C_{3/2} = 1/6$	$*C_{-5/2} = *1/3$
			2	$C_{9/2} = 5/12$	$C_{-7/2} = *1/12$	$*C_{5/2} = *1/3$	$*C_{-3/2} = 1/6$
2_8	${}^2_6 7'$	${}^2_6'$	1	$C_{7/2} = 5/96$	$C_{-1/2} = 7/16$	$C_{-9/2} = 1/96$	$*C_{11/2} = *11/32$
				$*C_{3/2} = *5/48$	$*C_{-5/2} = *5/96$		
			2	$C_{9/2} = 1/96$	$C_{1/2} = 7/16$	$C_{-7/2} = 5/96$	$*C_{5/2} = *1/24$
				$*C_{-3/2} = *5/48$	$*C_{11/2} = *11/32$		
	${}^2_7'$		1	$C_{7/2} = 5/96$	$C_{-1/2} = 7/16$	$C_{-9/2} = 1/96$	$*C_{11/2} = 11/32$
				$*C_{3/2} = 5/48$	$*C_{-5/2} = 5/96$		
			2	$C_{9/2} = 1/96$	$C_{1/2} = 7/16$	$C_{-7/2} = 5/96$	$*C_{5/2} = 1/24$
				$*C_{-3/2} = 5/48$	$*C_{11/2} = 11/32$		

$$S = 6 \quad D_6 = 2\Gamma'_1 + \Gamma'_{23} + 3\Gamma'_4$$

1	${}^1_1'$	1	$C_0 = *1/8$	$C_4 = 7/16$	$C_{-4} = 7/16$		
2	${}^2_1'$	1	$C_2 = *11/32$	$C_{-2} = *11/32$	$C_6 = 5/32$	$C_{-6} = 5/32$	
3	$23'$	$2'$	1	$C_0 = 7/16$	$C_4 = 1/32$	$C_{-4} = 1/32$	$*C_2 = 5/64$
				$*C_6 = 11/64$	$*C_{-6} = 11/64$		
	$3'$	1	$C_0 = 7/16$	$C_4 = 1/32$	$C_{-4} = 1/32$	$*C_2 = *5/64$	$*C_{-2} = *5/64$
				$*C_6 = *11/64$	$*C_{-6} = *11/64$		

$S = 13/2 \quad D_{13/2} = 3\Gamma'_5 + 2\Gamma'_{67}$

1_8	${}^1_{67'}$	${}^1_6'$	1	$C_{7/2} = 11/28 \quad C_{-9/2} = *3/28$ $*C_{11/2} = 169/772 \quad *C_{3/2} = *33/224 \quad *C_{-5/2} = 55/772 \quad *C_{-13/2} = *13/772$
			2	$C_{9/2} = 3/28 \quad C_{-7/2} = *11/28$ $*C_{13/2} = 33/772 \quad *C_{5/2} = *55/772 \quad *C_{-3/2} = 33/224 \quad *C_{-11/2} = *169/772$
		${}^1_7'$	1	$C_{7/2} = 11/28 \quad C_{-9/2} = *3/28$ $*C_{11/2} = *169/772 \quad *C_{3/2} = 33/224 \quad *C_{-5/2} = *55/772 \quad *C_{-13/2} = 13/772$
			2	$C_{9/2} = 3/28 \quad C_{-7/2} = *11/28$ $*C_{13/2} = *33/772 \quad *C_{5/2} = 55/772 \quad *C_{-3/2} = *33/224 \quad *C_{-11/2} = 169/772$
2_8	${}^2_{67'}$	${}^2_6'$	1	$C_{7/2} = *3/224 \quad C_{-1/2} = *7/16 \quad C_{-9/2} = *11/224$ $*C_{11/2} = 11/448 \quad *C_{3/2} = 25/448 \quad *C_{-5/2} = 45/448 \quad *C_{-13/2} = 143/448$
			2	$C_{9/2} = 11/224 \quad C_{1/2} = 7/16 \quad C_{-7/2} = 3/224$ $*C_{13/2} = *143/448 \quad *C_{5/2} = *45/448 \quad *C_{-3/2} = *25/448 \quad *C_{-11/2} = *11/448$
		${}^2_7'$	1	$C_{7/2} = *3/224 \quad C_{-1/2} = *7/16 \quad C_{-9/2} = *11/224$ $*C_{11/2} = *11/448 \quad *C_{3/2} = *25/448 \quad *C_{-5/2} = *45/448 \quad *C_{-13/2} = *143/448$
			2	$C_{9/2} = 11/224 \quad C_{1/2} = 7/16 \quad C_{-7/2} = 3/224$ $*C_{13/2} = 143/448 \quad *C_{5/2} = 45/448 \quad *C_{-3/2} = 25/448 \quad *C_{-11/2} = 11/448$

$S = 7 \quad D_7 = \Gamma'_1 + \Gamma'_{23} + 4\Gamma'_4$

3	${}^{23'}$	${}^2_7'$	1	$C_4 = 1/4 \quad C_{-4} = *1/4 \quad *C_2 = 11/96 \quad *C_{-2} = *11/96 \quad *C_6 = *13/96$ $*C_{-6} = 13/96$
		${}^3_7'$	1	$C_4 = 1/4 \quad C_{-4} = *1/4 \quad *C_2 = *11/96 \quad *C_{-2} = 11/96 \quad *C_6 = 13/96$ $*C_{-6} = *13/96$

$S = 15/2 \quad D_{15/2} = 2\Gamma'_5 + 3\Gamma'_{67}$

1_8	${}^1_{67'}$	${}^1_6'$	1	$C_{15/2} = 1001/3072 \quad C_{7/2} = *55/1024 \quad C_{-1/2} = *105/1024 \quad C_{-9/2} = *55/3072$ $*C_{3/2} = *5/16 \quad *C_{-5/2} = *3/16$
			2	$C_{9/2} = *55/3072 \quad C_{1/2} = *105/1024 \quad C_{-7/2} = *55/1024 \quad C_{-15/2} = 1001/3072$ $*C_{5/2} = *3/16 \quad *C_{-3/2} = *5/16$
		${}^1_7'$	1	$C_{15/2} = 1001/3072 \quad C_{7/2} = *55/1024 \quad C_{-1/2} = *105/1024 \quad C_{-9/2} = *55/3072$ $*C_{3/2} = 5/16 \quad *C_{-5/2} = 3/16$
			2	$C_{9/2} = *55/3072 \quad C_{1/2} = *105/1024 \quad C_{-7/2} = *55/1024 \quad C_{-15/2} = 1001/3072$ $*C_{5/2} = 3/16 \quad *C_{-3/2} = 5/16$

2_8	$^2_6 7'$	$^2_6'$	1	$C_{15/2} = 5/1024$	$C_{7/2} = 273/1024$	$C_{-1/2} = *143/1024$	$C_{-9/2} = 91/1024$
				$*C_{11/2} = *7/16$	$*C_{-13/2} = *1/16$		
		2	$C_{9/2} = 91/1024$	$C_{1/2} = *143/1024$	$C_{-7/2} = 273/1024$	$C_{-15/2} = 5/1024$	
			$*C_{13/2} = *1/16$	$*C_{-11/2} = *7/16$			
2_8	$^2_7'$	1	$C_{15/2} = 5/1024$	$C_{7/2} = 273/1024$	$C_{-1/2} = *143/1024$	$C_{-9/2} = 91/1024$	
				$*C_{11/2} = 7/16$	$*C_{-13/2} = 1/16$		
		2	$C_{9/2} = 91/1024$	$C_{1/2} = *143/1024$	$C_{-7/2} = 273/1024$	$C_{-15/2} = 5/1024$	
			$*C_{13/2} = 1/16$	$*C_{-11/2} = 7/16$			
3_8	$^3_6 7'$	$^3_6'$	1	$C_{7/2} = *1/8$	$C_{-9/2} = 3/8$		
				$*C_{11/2} = *13/384$	$*C_{3/2} = 11/128$	$*C_{-5/2} = *55/384$	$*C_{-13/2} = 91/384$
		2	$C_{9/2} = 3/8$	$C_{-7/2} = *1/8$			
			$*C_{13/2} = 91/384$	$*C_{5/2} = *55/384$	$*C_{-3/2} = 11/128$	$*C_{-11/2} = *13/384$	
	$^3_7'$	1	$C_{7/2} = *1/8$	$C_{-9/2} = 3/8$			
			$*C_{11/2} = 13/384$	$*C_{3/2} = *11/128$	$*C_{-5/2} = 55/384$	$*C_{-13/2} = *91/384$	
	2	$C_{9/2} = 3/8$	$C_{-7/2} = *1/8$				
		$*C_{13/2} = *91/384$	$*C_{5/2} = 55/384$	$*C_{-3/2} = *11/128$	$*C_{-11/2} = 13/384$		

$$S = 8 \quad D_8 = \Gamma'_1 + 2\Gamma'_{23} + 4\Gamma'_4$$

1_3	$^1_{23}'$	$^1_2'$	1	$C_8 = 5/2048$	$C_{-8} = 5/2048$	$C_4 = 91/512$	$C_{-4} = 91/512$	$C_0 = *143/1024$
				$*C_6 = 1/4$	$*C_{-6} = 1/4$			
	$^1_3'$	1	$C_8 = 5/2048$	$C_{-8} = 5/2048$	$C_4 = 91/512$	$C_{-4} = *91/512$	$C_0 = *143/1024$	
			$*C_6 = *1/4$	$*C_{-6} = *1/4$				
2_3	$^2_{23}'$	$^2_2'$	1	$C_8 = 1001/6144$	$C_{-8} = 1001/6144$	$C_4 = *55/1536$	$C_{-4} = *55/1536$	
				$C_0 = *105/1024$	$*C_2 = 1/4$	$*C_{-2} = 1/4$		
	$^2_3'$	1	$C_8 = 1001/6144$	$C_{-8} = 1001/6144$	$C_4 = *55/1536$	$C_{-4} = *55/1536$		
			$C_0 = *105/1024$	$*C_2 = *1/4$	$*C_{-2} = *1/4$			

$$S = 17/2 \quad D_{17/2} = 3\Gamma'_5 + 3\Gamma'_{67}$$

1_8	$^1_{67}'$	$^1_6'$	1	$C_{15/2} = 1001/55296$	$C_{7/2} = *275/13824$	$C_{-1/2} = *105/1024$	$C_{-9/2} = *715/13824$
				$C_{-17/2} = 17017/55296$	$*C_{3/2} = *7/36$	$*C_{-5/2} = *11/36$	
		2	$C_{17/2} = *17017/55296$	$C_{9/2} = 715/13824$	$C_{1/2} = 105/1024$	$C_{-7/2} = 275/13824$	
			$C_{-15/2} = *1001/3072$	$*C_{5/2} = 11/36$	$*C_{-3/2} = 7/36$		

Tables of functions transforming according to the irreducible representations of crystal point cubic T and T_h groups

${}^17'$	1	$C_{15/2} = 1001/55296$	$C_{7/2} = *275/13824$	$C_{-1/2} = *105/1024$	$C_{-9/2} = *715/13824$		
		$C_{-17/2} = 17017/55296$	$*C_{3/2} = 7/36$	$*C_{-5/2} = 11/36$			
	2	$C_{17/2} = *17017/55296$	$C_{9/2} = 715/13824$	$C_{1/2} = 105/1024$	$C_{-7/2} = 275/13824$		
		$C_{-15/2} = *1001/3072$	$*C_{5/2} = *11/36$	$*C_{-3/2} = *7/36$			
28	${}^267'$	${}^26'$	1	$C_{15/2} = 5/18432$	$C_{7/2} = 455/4608$	$C_{-1/2} = *143/1024$	$C_{-9/2} = 1183/4608$
				$C_{-17/2} = 85/18432$	$*C_{11/2} = *1/12$	$*C_{-13/2} = *5/12$	
			2	$C_{17/2} = *85/18432$	$C_{9/2} = *1183/4608$	$C_{1/2} = 143/1024$	$C_{-7/2} = *455/4608$
				$C_{-15/2} = *5/18432$	$*C_{13/2} = 5/12$	$*C_{-11/2} = 1/12$	
${}^27'$	1		$C_{15/2} = 5/18432$	$C_{7/2} = 455/4608$	$C_{-1/2} = *143/1024$	$C_{-9/2} = 1183/4608$	
			$C_{-17/2} = 85/18432$	$*C_{11/2} = 1/12$	$*C_{-13/2} = 5/12$		
	2		$C_{17/2} = *85/18432$	$C_{9/2} = *1183/4608$	$C_{1/2} = 143/1024$	$C_{-7/2} = *455/4608$	
			$C_{-15/2} = *5/18432$	$*C_{13/2} = *5/12$	$*C_{-11/2} = *1/12$		
38	${}^367'$	${}^36'$	1	$C_{15/2} = *289/864$	$C_{7/2} = *91/864$	$C_{-9/2} = 35/864$	$C_{-17/2} = 17/864$
				$*C_{11/2} = *5/64$	$*C_{3/2} = *143/576$	$*C_{-5/2} = 91/576$	$*C_{-13/2} = 1/64$
	2		$C_{17/2} = *17/864$	$C_{9/2} = *35/864$	$C_{-7/2} = 91/864$	$C_{-15/2} = 289/864$	
			$*C_{13/2} = *1/64$	$*C_{5/2} = *91/576$	$*C_{-3/2} = 143/576$	$*C_{-11/2} = 5/64$	
${}^37'$	1		$C_{15/2} = *289/864$	$C_{7/2} = *91/864$	$C_{-9/2} = 35/864$	$C_{-17/2} = 17/864$	
			$*C_{11/2} = 5/64$	$*C_{3/2} = 143/576$	$*C_{-5/2} = *91/576$	$*C_{-13/2} = *1/64$	
	2		$C_{17/2} = *17/864$	$C_{9/2} = *35/864$	$C_{-7/2} = 91/864$	$C_{-15/2} = 289/864$	
			$*C_{13/2} = 1/64$	$*C_{5/2} = 91/576$	$*C_{-3/2} = *143/576$	$*C_{-11/2} = *5/64$	

The functions transforming according to IR Γ'_1 , Γ'_4 , and Γ'_5 of T , T' and T_h , T'_h groups were already given in [14].

Conclusion

Tables of functions transforming according to Γ'_{23} and Γ'_{67} representations of T , T' and T_h , T'_h cubic groups are given. The functions obtained by projecting IR D_S of the rotation group on subspaces of IR Γ'_2 , Γ'_3 and Γ'_6 , Γ'_7 of T , T' and T_h , T'_h cubic groups are simply united into Γ'_{23} and Γ'_{67} representations. Such functions contain all the information that distinguishes T , T' and T_h , T'_h groups from O , O' , T_d , T'_d and O_h , O'_h groups of the higher cubic symmetry, and make it possible to consider the effects due to the additional term of the six-order CEF potential.

Acknowledgments

I am grateful to M.V. Eremin, who drew my attention to the problem under discussion, and also for the critical use of Tables [14]. This work was funded by the subsidy allocated to Kazan Federal University for the state assignment in the sphere of scientific activities (project 3.672.2017/8.9).

References

1. Chakoumakos B.C., Sales B.C. *J. Alloys Compd.* **407**, 87 (2006).
2. Aoki Y., Namiki T., Matsuda T.D., Abe K., Sugawara H., Sato H. *Phys. Rev. B* **65**, 064446 (2002).
3. Sugawara H., Matsuda T.D., Abe K., Aoki Y., Sato H., Nojiri S., Inada Y., Settai R., Onuki Y. *Phys. Rev. B* **66**, 134411 (2002).
4. Sekine S., Uchiumi T., Shirotani I., Yagi T. *Phys. Rev. Lett.* **79**, 3218 (1997).
5. Matsunami M., Chen L., Okamura H., Nanba T., Sekine S., Shirotani I. *J. Magn. Mater.* **272-276**, E39 (2004).
6. Yogi M., Kotegawa H., Imamura Y., Zheng G.-Q., Kitaoka Y., Sugawara H., Sato H. *Phys. Rev. B* **67**, 180501 (2003).
7. Bauer E.D., Frederick N.A., Ho P.-C., Zapf V.S., Maple M.B. *Phys. Rev. B* **65**, 100506 (2002).
8. Maple M.B., Bauer E.D., Zapf V.S., Freeman E.J., Frederick N.A., Dickey R.P. *Acta Phys. Pol. B* **32**, 3291 (2001).
9. Bauer E.D., Berger S., Paul C., Della Mea M., Hilscher G., Michor H., Reissner M., Steiner W., Grytsiv A., Rogl P., Scheidt E.W. *Phys. Rev. B* **66**, 214421 (2002).
10. Butch N.P., Yuhasz W.M., Ho P.-C., Jeffries J.R., Frederick N.A., Sayles T.A., Zheng X.G., Maple M.B., Betts J.B., Lacerda A.H., Woodward F.M., Lynn J.W., Rogl P., Giester G. *Phys. Rev. B* **71**, 214417 (2005).
11. Yuhasz W.M., Butch N.P., Sayles T.A., Ho P.-C., Jeffries J.R., Yanagisawa T., Frederick N.A., Maple M.B., Henkie Z., Pietraszko A., McCall S.K., McElfresh M.W., Fluss M.J. *Phys. Rev. B* **73**, 144409 (2006).
12. Maple M.B., Butch N.P., Frederick N.A., Ho P.-C., Jeffries J.R., Sayles T.A., Yanagisawa T., Yuhasz W.M., Songxue Chi, Kang H.J., Lynn J.W., Dai Pengcheng, McCall S.K., McElfresh M.W., Fluss M.J., Henkie Z., Pietraszko A. *Proc. Natl. Acad. Sci. USA*. **103**, 6783 (2006).
13. Adroja D.T., Park J.-G., Goremychkin E.A., Takeda N., Ishikawa M., McEwen K.A., Osborn R., Hillier A.D., Rainford B.D. *Physica B* **359-361**, 983 (2005).
14. Leushin A.M. *Tables of Functions Transforming According to the Irreducible Representations of Crystal Point Groups*, Nauka, Moscow (1968), 143 p. (in Russian).
15. Koster G.F., Dimmock J.O., Wheeler R.G., Statz H. *Properties of the Thirty-Two Point Groups*, The M.I.T. Press, Cambridge, Massachusetts (1963), 104 p.
16. Bethe H.A. *Ann. d. Phys.* **3**, 133 (1929).
17. Takegahara K., Harima H., Yanase A. *J. Phys. Soc. Japan* **70**, 1190 (2001).
18. Park J.-G., Adroja D.T., McEwen K.A., Kohgi M., Iwasa K. *Phys. Rev. B* **77**, 085102 (2008).
19. Chi Sengxue, Dai Pengcheng, Barnes T., Kang H.J., Lynn J.W., Bewley R., Ye F., Maple M.B., Henkie Z., Pietraszko A. *Phys. Rev. B* **77**, 094428 (2008).
20. Garcia D.J., Garcia F.A., Duque J.G.S., Pagliuso P.G., Rettori C., Schlottmann P., Torikachvili M.S., Oseroff S.B. *Phys. Rev. B* **78** 174428 (2008).
21. Garcia F.A., Garcia D.J., Avila M.A., Vargas J.M., Pagliuso P.G., Rettori C., Passeggi M.C.G., Oseroff S.B., Schlottmann P., Alascio B., Fisk Z. *Phys. Rev. B* **80**, 052401 (2009).
22. Goremychkin E.A., Osborn R., Bauer E.D., Maple M.B., Frederick N.A., Yuhasz W.M., Woodward F.M., Lynn J.W. *Phys. Rev. Lett.* **93**, 157003 (2004).
23. Landau L.D., Lifshitz E.M. *Quantum Mechanics – Non Relativistic Theory*, Addison-Wesley Publishing Co., Inc., Reading, Mass. (1958), 338 p.