Supporting Information

Symmetry analysis of complex magnetic structure in monoclinically distorted $Er_3Cu_4Sn_4$

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The Supporting Information contains symmetry analysis of allowed magnetic structures in $Er_3Cu_4Sn_4$ as generated by the BasIreps computer program.

TABLE OF CONTENTS

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  +++ PROGRAM:BasIreps (Version 4.10, November 2012)+++
  +++                  (JRC- ILL)                   +++
  +++++++++++++++++++++++++++++++++++++++++++++++++++++++

 The calculation of the IRREPS of the little group is based in
 the procedure of ZAK provided within the program KAREP
 E. Hovestreydt, I. Aroyo et al, J.Appl.Cryst. 25, 544 (1992)
 Program based in CrysFML (Crystallographic Fortran-95 Modules Library)
 BasIreps -> (Version 4.10, November 2012), ILL-Juan Rodriguez-Carvajal

=> Title:Test of new BASIREPS
=> Symbol of the space group: C 2/m
=> The given space group C 2/m is standard, IT generators will be used
=> List of space group generators:  x+1/2,y+1/2,z; -x,y,-z; -x,-y,-z
=> Propagation vector:   0.0000  0.0000  0.5000
=> BZ-point labelled as  G
=> The representations of Gk will be calculated



       Information on Space Group:
       ---------------------------

=>   Number of Space group:  12
=>  Hermann-Mauguin Symbol: C 2/m
=>             Hall Symbol: -C 2y
=>    Table Setting Choice: b1
=>            Setting Type: Generated from explicit IT generators
=>          Crystal System: Monoclinic
=>              Laue Class: 2/m
=>             Point Group: 2/m
=>         Bravais Lattice: C
=>          Lattice Symbol: mC
=>  Reduced Number of S.O.:   2
=>    General multiplicity:   8
=>          Centrosymmetry: Centric (-1 at origin)
=>  Generators (exc. -1&L):   1
=>         Asymmetric unit:  0.000 <= x <=  0.500
                             0.000 <= y <=  0.250
                             0.000 <= z <=  1.000
=> Centring vectors:  1
=> Latt( 1): (1/2,1/2,0)

=> List of all Symmetry Operators and Symmetry Symbols

=> SYMM(  1): x,y,z                              Symbol: 1
=> SYMM(  2): -x,y,-z                            Symbol: 2 0,y,0
=> SYMM(  3): -x,-y,-z                           Symbol: -1 0,0,0
=> SYMM(  4): x,-y,z                             Symbol: m x,0,z
=> SYMM(  5): x+1/2,y+1/2,z                      Symbol: t (1/2,1/2,0)
=> SYMM(  6): -x+1/2,y+1/2,-z                    Symbol: 2 (0,1/2,0) 1/4,y,0
=> SYMM(  7): -x+1/2,-y+1/2,-z                   Symbol: -1 1/4,1/4,0
=> SYMM(  8): x+1/2,-y+1/2,z                     Symbol: a x,1/4,z

=> Special Wyckoff Positions for C 2/m

   Multp     Site        Representative Coordinates (centring translations excluded)
     4       i              x,0,z               -x,0,-z

     4       h              0,y,1/2             0,-y,1/2

     4       g              0,y,0               0,-y,0

     4       f              1/4,1/4,1/2         3/4,1/4,1/2

     4       e              1/4,1/4,0           3/4,1/4,0

     2       d              0,1/2,1/2
```

```
     2       c              0,0,1/2

     2       b              0,1/2,0

     2       a              0,0,0


 => Number of generators of space group:   2

 GEN(1): -x,y,-z
 GEN(2): -x,-y,-z

  TRANSLATIONAL COSET REPRESENTATIVES OF SPACE GROUP: C 2/m

  Num          Symmetry-Element                  Eqv. Positions
-------------------------------------------------------------
(  1)   1                                       x,y,z
(  2)   2 0,y,0                                 -x,y,-z
(  3)   -1 0,0,0                                -x,-y,-z
(  4)   m x,0,z                                 x,-y,z


 => The lattice symbol is mC


  The conventional k-vector is
     0.00000     0.00000     0.50000

 THE GENERATORS OF THE LITTLE GROUP OF BRILLOUIN ZONE POINT  G

 The little group can be generated from the following 2 elements:-

  => GENk(1): -x,y,-z
  => GENk(2): -x,-y,-z

 REPRESENTATIVE ELEMENTS OF THE LITTLE GROUP OF BRILLOUIN ZONE POINT  G

  Operator of Gk Number( 1): x,y,z
  Operator of Gk Number( 2): -x,y,-z
  Operator of Gk Number( 3): -x,-y,-z
  Operator of Gk Number( 4): x,-y,z

 ------------------------------------------------------------
 => Number of elements of G_k:   4
 => Number of irreducible representations of G_k:   4
 => Dimensions:  1 1 1 1

 => Symmetry elements of G_k and irreps:
    Symmetry elements reduced to the standard form (positive translations < 1)
    The matrices of IRreps have been multiplied by the appropriate phase factor

 -> SYMM_K( 1):  x,y,z                   :   1            ->  h1           Int. symbol: 1
    Phase factor for correcting input data:  0.0000
    Matrix of IRrep( 1):
                     1
    Matrix of IRrep( 2):
                     1
    Matrix of IRrep( 3):
                     1
    Matrix of IRrep( 4):
                     1
 -> SYMM_K( 2):  -x,y,-z                 :   2 ( 0, y, 0) ->  h3           Int. symbol: 2
0,y,0
    Phase factor for correcting input data:  0.0000
    Matrix of IRrep( 1):
                     1
    Matrix of IRrep( 2):
                     1
    Matrix of IRrep( 3):
                    -1
    Matrix of IRrep( 4):
                    -1
 -> SYMM_K( 3):  -x,-y,-z                :  -1            -> h25           Int. symbol: -1
0,0,0
```

```
    Phase factor for correcting input data:  0.0000
    Matrix of IRrep( 1):
                      1
    Matrix of IRrep( 2):
                     -1
    Matrix of IRrep( 3):
                      1
    Matrix of IRrep( 4):
                     -1
 -> SYMM_K( 4):  x,-y,z                  :   m ( x, 0, z) -> h27          Int. symbol: m
x,0,z
    Phase factor for correcting input data:  0.0000
    Matrix of IRrep( 1):
                      1
    Matrix of IRrep( 2):
                     -1
    Matrix of IRrep( 3):
                     -1
    Matrix of IRrep( 4):
                      1


    ============================================================================
    Writing of Irreps matrices in symbolic form:  Module:Phase (fractions of 2pi)
    Numeric values of symbols a,b,c,d, ... are given at the end of the table
    ============================================================================

   In this section the translations associated to Seitz symbols are simplified as
      1/2  1/3  2/3  1/4  3/4  1/6  5/6  1/8  3/8  5/8  7/8
        p    q    r    s    t    u    v    w    x    y    z

    The rotational part of Seitz symbols contains information about the orientation as
   defined in Kovalev. The international symbols may be truncated (for format reasons) in
   the table below. The complete international symbols can be found in the previous list.
-------------------------------------------------------------------------
  Ireps               Symmetry operators ->
    v     1             2 0,y,0       -1 0,0,0      m x,0,z
    v     {1|000}       {2_0y0|000}   {-1|000}      {m_x0z|000}
    v        Symm( 1)      Symm( 2)      Symm( 3)      Symm( 4)
-------------------------------------------------------------------------


 IRrep( 1):     1             1             1             1


 IRrep( 2):     1             1            -1            -1


 IRrep( 3):     1            -1             1            -1


 IRrep( 4):     1            -1            -1             1


 ---------------------------------------------------------------
 List of constants and phase factors defined in the above table
 ---------------------------------------------------------------

 The propagation vector is k=( 0.00000, 0.00000, 0.50000)


 => Alternative evaluation of the propagation vector group.
    The ordering of the symmetry operators may be different
    than the sequence numbering given above
    ---------------------------------------------------------

      PROPAGATION VECTOR GROUP INFORMATION
      ====================================

 => The input propagation vector is: K=(  0.0000  0.0000  0.5000 )
 => K .. IS .. equivalent to -K
 => The operators following the k-vectors constitute the co-set decomposition G[Gk]
    The list of equivalent k-vectors are also given on the right of operators.
 => The star of K is formed by the following   1 vectors:
```

```
  Eqv. -K: k_1  = (  0.0000  0.0000  0.5000 )    Op: (  1) x,y,z
                                                 Op: (  2) -x,y,-z           -> (   0.0000
0.0000 -0.5000 )
                                                 Op: (  3) -x,-y,-z          -> (   0.0000
0.0000 -0.5000 )
                                                 Op: (  4) x,-y,z            -> (   0.0000
0.0000  0.5000 )

 => G_k has the following symmetry operators:

      1 SYMM(  1) = x,y,z
      2 SYMM(  2) = -x,y,-z
      3 SYMM(  3) = -x,-y,-z
      4 SYMM(  4) = x,-y,z


      DATA ABOUT ATOMS
      ================


 => No. of sites:    1

 => Calculation for axial vectors

 => List of atoms within a primitive unit cell:
                X       Y       Z           for site:  1
 -> Er1_1   :   0.0000  0.0000  0.5000  : (x,y,z)


     CALCULATIONS FOR SITE : 1

================================================================================
       Sym.Op.     Atoms Numbers, phases and returning Vectors
      Vector Rep.    Character(V)    Character(Perm)(r,i)  ChM
================================================================================
 SYMM_K( 1): x,y,z                          :   1            ->  h1
       Atoms:          1
       Phase:          +
      Vector:     0.0 0.0 0.0
      Vector Representation: ( Mx, My, Mz)
      Ch(V):  3.0  Chr(P):  1.0  Chr(T):  3.0
--------------------------------------------------------------------------------
 SYMM_K( 2): -x,y,-z                        :   2 ( 0, y, 0) ->  h3
       Atoms:          1
       Phase:          -
      Vector:     0.0 0.0 1.0
      Vector Representation: (-Mx, My,-Mz)
      Ch(V): -1.0  Chr(P): -1.0  Chr(T):  1.0
--------------------------------------------------------------------------------
 SYMM_K( 3): -x,-y,-z                       :  -1            -> h25
       Atoms:          1
       Phase:          -
      Vector:     0.0 0.0 1.0
      Vector Representation: ( Mx, My, Mz)
      Ch(V):  3.0  Chr(P): -1.0  Chr(T): -3.0
--------------------------------------------------------------------------------
 SYMM_K( 4): x,-y,z                         :   m ( x, 0, z) -> h27
       Atoms:          1
       Phase:          +
      Vector:     0.0 0.0 0.0
      Vector Representation: (-Mx, My,-Mz)
      Ch(V): -1.0  Chr(P):  1.0  Chr(T): -1.0
--------------------------------------------------------------------------------

 => Decomposition of the Magnetic/Mechanic representation:

 -> Characters of GAMMA and IRreps:

  GAMMA       G( 1)    G( 2)    G( 3)    G( 4)
            3.0 0.0  1.0 0.0 -3.0 0.0 -1.0 0.0

Irep_k( 1)    G( 1)    G( 2)    G( 3)    G( 4)
            1.0 0.0  1.0 0.0  1.0 0.0  1.0 0.0

Irep_k( 2)    G( 1)    G( 2)    G( 3)    G( 4)
```

```
            1.0 0.0  1.0 0.0 -1.0 0.0 -1.0 0.0

Irep_k( 3)    G( 1)    G( 2)    G( 3)    G( 4)
            1.0 0.0 -1.0 0.0  1.0 0.0 -1.0 0.0

Irep_k( 4)    G( 1)    G( 2)    G( 3)    G( 4)
            1.0 0.0 -1.0 0.0 -1.0 0.0  1.0 0.0

 -> GAMMA(Magnetic):   2 Irep_k( 2) + 1 Irep_k( 4)

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 => Decomposition of the Permutational Representation:

 -> GAMMA(Permutation):   1 Irep_k( 4)

 => Exchange multiplets:

    Representation Irep_k( 4) x Axial:   2 Irep_k( 2) + 1 Irep_k( 4)

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-------------------------------------------------------------------------------------------------
                     General information relating the calculated basis functions with the
magnetic structure

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       The fundamental hypothesis of the representational analysis is that the vectorial
Fourier coefficients are
       LINEAR COMBINATIONS of Basis Functions, in a simplified form: Sk(j) = Sum{n}
{C(n).BsV(n,j)}
       The index 'j' labels the sublatices (j=1,2,...na) of the current site: Er1_1
       The simplified notation for C(n) used below, is given by the symbols: u,v,w,p,q ....
(may be complex!)
       The Fourier coefficients are written as: Sk(j) = u BsV(1,j)+ v BsV(2,j)+ w BsV(3,j)+ p
BsV(4,j)+ q BsV(5,j)+ ...
       The atomic components of the basis functions BsV(n,j) are 3D constant vectors (may be
complex) written as row matrices
       BsV(n,j) represents the basis vector 'n' attached to the atom 'j'
       BsV(n,1:na) represents the basis vectors 'n' of the atoms 1 up to na (row of na 3D-
vectors)
       The magnetic moments should be calculated from the Fourier coefficients using the
general formula:

                                  m(L,j) = Sum{k}{ Sk(j) exp[-2pi.i.k.R(L)] }

       or for a single pair (k,-k)

                                  m(L,j) = Sk(j) exp{-2pi.i.k.R(L)} +  Sk*(j) exp{2pi.i.k.R(L)}

       Where R(L) is the LATTICE translation giving the vector position of the cell labelled
'L':  R(L) = L1 a + L2 b + L3 c

       If the lattice is CENTRED the expression of R(L) contains also fractional indices
(L1,L2,L3)
       The components of m(L,j), Sk(j) and BsV(n,j) are given with respect to a frame with
unit vectors along a,b,c

       In the present case k = ( 0.00000, 0.00000, 0.50000) is equivalent to -k and all Sk(j)
should be real
       Up to a sign, the magnetic moments are identified to the Fourier coefficients Sk(j):
m(L,j) = Sk(j)(-1)^{0 L1 + 0 L2 + 1 L3 }

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 => Atomic components of the BASIS FUNCTIONS using PROJECTION OPERATORS:
                   Calculation for SITE number:  1
               (Only non-null functions are written)


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 => Basis functions of Representation IRrep( 2) of dimension  1 contained 2 times in GAMMA
   ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

              SYMM  x,y,z
              Atoms:      Er1_1
 BsV( 1, 1: 1):Re (    1    0    0)
 BsV( 2, 1: 1):Re (    0    0    1)


 ----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients
u,v,w,p,q ....(may be complex!)

       The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
       by lattice translations are the following:

       SYMM x,y,z                                                        Atom: Er1_1
0.0000  0.0000  0.5000
       Sk(1): (u,0,v)

   ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 => Basis functions of Representation IRrep( 4) of dimension  1 contained 1 times in GAMMA
   ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

              SYMM  x,y,z
              Atoms:      Er1_1
 BsV( 1, 1: 1):Re (    0    1    0)


 ----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients
u,v,w,p,q ....(may be complex!)

       The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
       by lattice translations are the following:

       SYMM x,y,z                                                        Atom: Er1_1
0.0000  0.0000  0.5000
       Sk(1): (0,u,0)
-------------------------------------------------------------------------------
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  +++ PROGRAM:BasIreps (Version 4.10, November 2012)+++
  +++                  (JRC- ILL)                   +++
  +++++++++++++++++++++++++++++++++++++++++++++++++++++++

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 Program based in CrysFML (Crystallographic Fortran-95 Modules Library)
 BasIreps -> (Version 4.10, November 2012), ILL-Juan Rodriguez-Carvajal

=> Title:Test of new BASIREPS
=> Symbol of the space group: C 2/m
=> The given space group C 2/m is standard, IT generators will be used
=> List of space group generators:  x+1/2,y+1/2,z; -x,y,-z; -x,-y,-z
=> Propagation vector:   1.0000  0.4667  0.5000
=> BZ-point labelled as  G
=> The representations of Gk will be calculated



       Information on Space Group:
       ---------------------------

=>   Number of Space group:  12
=>  Hermann-Mauguin Symbol: C 2/m
=>             Hall Symbol: -C 2y
=>    Table Setting Choice: b1
=>            Setting Type: Generated from explicit IT generators
=>          Crystal System: Monoclinic
=>              Laue Class: 2/m
=>             Point Group: 2/m
=>         Bravais Lattice: C
=>          Lattice Symbol: mC
=>  Reduced Number of S.O.:   2
=>    General multiplicity:   8
=>          Centrosymmetry: Centric (-1 at origin)
=>  Generators (exc. -1&L):   1
=>         Asymmetric unit:  0.000 <= x <=  0.500
                             0.000 <= y <=  0.250
                             0.000 <= z <=  1.000
=> Centring vectors:  1
=> Latt( 1): (1/2,1/2,0)

=> List of all Symmetry Operators and Symmetry Symbols

=> SYMM(  1): x,y,z                              Symbol: 1
=> SYMM(  2): -x,y,-z                            Symbol: 2 0,y,0
=> SYMM(  3): -x,-y,-z                           Symbol: -1 0,0,0
=> SYMM(  4): x,-y,z                             Symbol: m x,0,z
=> SYMM(  5): x+1/2,y+1/2,z                      Symbol: t (1/2,1/2,0)
=> SYMM(  6): -x+1/2,y+1/2,-z                    Symbol: 2 (0,1/2,0) 1/4,y,0
=> SYMM(  7): -x+1/2,-y+1/2,-z                   Symbol: -1 1/4,1/4,0
=> SYMM(  8): x+1/2,-y+1/2,z                     Symbol: a x,1/4,z

=> Special Wyckoff Positions for C 2/m

   Multp     Site        Representative Coordinates (centring translations excluded)
     4       i              x,0,z               -x,0,-z

     4       h              0,y,1/2             0,-y,1/2

     4       g              0,y,0               0,-y,0

     4       f              1/4,1/4,1/2         3/4,1/4,1/2

     4       e              1/4,1/4,0           3/4,1/4,0

     2       d              0,1/2,1/2
```

```
     2       c              0,0,1/2

     2       b              0,1/2,0

     2       a              0,0,0


 => Number of generators of space group:   2

 GEN(1): -x,y,-z
 GEN(2): -x,-y,-z

  TRANSLATIONAL COSET REPRESENTATIVES OF SPACE GROUP: C 2/m

  Num          Symmetry-Element                  Eqv. Positions
 ------------------------------------------------------------
 (  1)   1                                      x,y,z
 (  2)   2 0,y,0                                -x,y,-z
 (  3)   -1 0,0,0                               -x,-y,-z
 (  4)   m x,0,z                                x,-y,z


 => The lattice symbol is mC


  The conventional k-vector is
     1.00000     0.46670     0.50000

 THE GENERATORS OF THE LITTLE GROUP OF BRILLOUIN ZONE POINT  G

 The little group can be generated from the following elements:

  => GENk(1): -x,y,-z

 REPRESENTATIVE ELEMENTS OF THE LITTLE GROUP OF BRILLOUIN ZONE POINT  G

  Operator of Gk Number( 1): x,y,z
  Operator of Gk Number( 2): -x,y,-z

 ------------------------------------------------------------
 => Number of elements of G_k:   2
 => Number of irreducible representations of G_k:   2
 => Dimensions:  1 1

 => Symmetry elements of G_k and irreps:
    Symmetry elements reduced to the standard form (positive translations < 1)
    The matrices of IRreps have been multiplied by the appropriate phase factor

 -> SYMM_K( 1):  x,y,z                    :   1           ->  h1          Int. symbol: 1
    Phase factor for correcting input data:  0.0000
    Matrix of IRrep( 1):
                      1
    Matrix of IRrep( 2):
                      1
 -> SYMM_K( 2):  -x,y,-z                  :   2 ( 0, y, 0) ->  h3          Int. symbol: 2
0,y,0
    Phase factor for correcting input data:  0.0000
    Matrix of IRrep( 1):
                      1
    Matrix of IRrep( 2):
                     -1


    ============================================================================
    Writing of Irreps matrices in symbolic form:  Module:Phase (fractions of 2pi)
    Numeric values of symbols a,b,c,d, ... are given at the end of the table
    ============================================================================

   In this section the translations associated to Seitz symbols are simplified as
      1/2  1/3  2/3  1/4  3/4  1/6  5/6  1/8  3/8  5/8  7/8
        p    q    r    s    t    u    v    w    x    y    z

    The rotational part of Seitz symbols contains information about the orientation as
```

```
   defined in Kovalev. The international symbols may be truncated (for format reasons) in
   the table below. The complete international symbols can be found in the previous list.
----------------------------------------
  Ireps               Symmetry operators ->
    v     1             2 0,y,0
    v     {1|000}       {2_0y0|000}
    v        Symm( 1)      Symm( 2)
----------------------------------------


 IRrep( 1):     1             1


 IRrep( 2):     1            -1


 ---------------------------------------------------------------
 List of constants and phase factors defined in the above table
 ---------------------------------------------------------------

 The propagation vector is k=( 1.00000, 0.46670, 0.50000)


 => Alternative evaluation of the propagation vector group.
    The ordering of the symmetry operators may be different
    than the sequence numbering given above
    ---------------------------------------------------------

      PROPAGATION VECTOR GROUP INFORMATION
      ====================================

 => The input propagation vector is: K=(  1.0000  0.4667  0.5000 )
 => K .. IS NOT .. equivalent to -K
 => The operators following the k-vectors constitute the co-set decomposition G[Gk]
    The list of equivalent k-vectors are also given on the right of operators.
 => The star of K is formed by the following   2 vectors:


           k_1  = (  1.0000  0.4667  0.5000 )    Op: (  1) x,y,z
                                                 Op: (  2) -x,y,-z           -> (  -1.0000
0.4667 -0.5000 )

  Eqv. -K: k_2  = ( -1.0000 -0.4667 -0.5000 )    Op: (  3) -x,-y,-z
                                                 Op: (  4) x,-y,z            -> (   1.0000 -
0.4667  0.5000 )

 => G_k has the following symmetry operators:

      1 SYMM(  1) = x,y,z
      2 SYMM(  2) = -x,y,-z


      DATA ABOUT ATOMS
      ================


 => No. of sites:    1

 => Calculation for axial vectors

 => List of atoms within a primitive unit cell:
                 X       Y       Z           for site:  1
 -> Er2_1   :   0.1299  0.0000  0.1177  : (x,y,z)
 -> Er2_2   :   0.8701  0.0000  0.8823  : (-x,y,-z) + (1,0,1)


     CALCULATIONS FOR SITE : 1

================================================================================
       Sym.Op.     Atoms Numbers, phases and returning Vectors
      Vector Rep.    Character(V)    Character(Perm)(r,i)  ChM
================================================================================
 SYMM_K( 1): x,y,z                          :   1            ->  h1
       Atoms:          1              2
       Phase:       0.0000         0.0000
```

```
      Vector:     0.0 0.0 0.0     0.0 0.0 0.0
      Vector Representation: ( Mx, My, Mz)
      Ch(V):  3.000 Chr(P):  2.000 Chi(P):  0.000 Chr(T):  6.000 Chi(T):  0.000
-------------------------------------------------------------------------------
 SYMM_K( 2): -x,y,-z                       :   2 ( 0, y, 0) ->  h3
       Atoms:          2              1
       Phase:       1.5000          1.5000
      Vector:     1.0 0.0 1.0     1.0 0.0 1.0
      Vector Representation: (-Mx, My,-Mz)
      Ch(V): -1.000 Chr(P):  0.000 Chi(P):  0.000 Chr(T):  0.000 Chi(T):  0.000
-------------------------------------------------------------------------------

 => Decomposition of the Magnetic/Mechanic representation:

 -> Characters of GAMMA and IRreps:

  GAMMA       G( 1)    G( 2)
            6.0 0.0  0.0 0.0

Irep_k( 1)    G( 1)    G( 2)
            1.0 0.0  1.0 0.0

Irep_k( 2)    G( 1)    G( 2)
            1.0 0.0 -1.0 0.0

 -> GAMMA(Magnetic):   3 Irep_k( 1) + 3 Irep_k( 2)

-------------------------------------------------------------------------------

 => Decomposition of the Permutational Representation:

 -> GAMMA(Permutation):   1 Irep_k( 1) + 1 Irep_k( 2)

 => Exchange multiplets:

    Representation Irep_k( 1) x Axial:   1 Irep_k( 1) + 2 Irep_k( 2)

    Representation Irep_k( 2) x Axial:   2 Irep_k( 1) + 1 Irep_k( 2)

-------------------------------------------------------------------------------


-------------------------------------------------------------------------------------------------
                     General information relating the calculated basis functions with the
magnetic structure

-------------------------------------------------------------------------------------------------

       The fundamental hypothesis of the representational analysis is that the vectorial
Fourier coefficients are
       LINEAR COMBINATIONS of Basis Functions, in a simplified form: Sk(j) = Sum{n}
{C(n).BsV(n,j)}
       The index 'j' labels the sublatices (j=1,2,...na) of the current site: Er2_1 Er2_2
       The simplified notation for C(n) used below, is given by the symbols: u,v,w,p,q ....
(may be complex!)
       The Fourier coefficients are written as: Sk(j) = u BsV(1,j)+ v BsV(2,j)+ w BsV(3,j)+ p
BsV(4,j)+ q BsV(5,j)+ ...
       The atomic components of the basis functions BsV(n,j) are 3D constant vectors (may be
complex) written as row matrices
       BsV(n,j) represents the basis vector 'n' attached to the atom 'j'
       BsV(n,1:na) represents the basis vectors 'n' of the atoms 1 up to na (row of na 3D-
vectors)
       The magnetic moments should be calculated from the Fourier coefficients using the
general formula:

                                  m(L,j) = Sum{k}{ Sk(j) exp[-2pi.i.k.R(L)] }

       or for a single pair (k,-k)

                                  m(L,j) = Sk(j) exp{-2pi.i.k.R(L)} +  Sk*(j) exp{2pi.i.k.R(L)}

       Where R(L) is the LATTICE translation giving the vector position of the cell labelled
'L':  R(L) = L1 a + L2 b + L3 c
```

```
       If the lattice is CENTRED the expression of R(L) contains also fractional indices
(L1,L2,L3)
       The components of m(L,j), Sk(j) and BsV(n,j) are given with respect to a frame with
unit vectors along a,b,c

       We consider only the propagation vector pair (k,-k) with k = ( 1.00000, 0.46670,
0.50000)

-------------------------------------------------------------------------------

 => Atomic components of the BASIS FUNCTIONS using PROJECTION OPERATORS:
                    Calculation for SITE number:  1
                (Only non-null functions are written)


   +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 => Basis functions of Representation IRrep( 1) of dimension  1 contained 3 times in GAMMA
   +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

              SYMM  x,y,z   -x+1,y,-z+1
              Atoms:      Er2_1             Er2_2
 BsV( 1, 1: 2):Re (    1    0    0) (    1    0    0)
 BsV( 2, 1: 2):Re (    0    1    0) (    0   -1    0)
 BsV( 3, 1: 2):Re (    0    0    1) (    0    0    1)


 ----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients
u,v,w,p,q ....(may be complex!)

       The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
       by lattice translations are the following:

       SYMM x,y,z                                                          Atom: Er2_1
0.1299  0.0000  0.1177
       Sk(1): (u,v,w)

       SYMM -x+1,y,-z+1                                                    Atom: Er2_2
0.8701  0.0000  0.8823
       Sk(2): (u,-v,w)

   +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 => Basis functions of Representation IRrep( 2) of dimension  1 contained 3 times in GAMMA
   +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

              SYMM  x,y,z   -x+1,y,-z+1
              Atoms:      Er2_1             Er2_2
 BsV( 1, 1: 2):Re (    1    0    0) (   -1    0    0)
 BsV( 2, 1: 2):Re (    0    1    0) (    0    1    0)
 BsV( 3, 1: 2):Re (    0    0    1) (    0    0   -1)


 ----- The Fourier coefficients are LINEAR COMBINATIONS of Basis Functions: coefficients
u,v,w,p,q ....(may be complex!)

       The general expressions of the Fourier coefficients Sk(j) of the atoms non-related
       by lattice translations are the following:

       SYMM x,y,z                                                          Atom: Er2_1
0.1299  0.0000  0.1177
       Sk(1): (u,v,w)

       SYMM -x+1,y,-z+1                                                    Atom: Er2_2
0.8701  0.0000  0.8823
       Sk(2): (-u,v,-w)
-------------------------------------------------------------------------------
```