## Example 2:

### *k=(0,0,1/2)* – space group No. 62 (P n m a) – pos. 4d

*For that case symmetry analysis shows:*

- two representations $\tau_1$ and $\tau_2$, both 3-dimensional,
- occurring two times each in the decomposition of magnetic representation.
- all atomic positions belong to one orbit of $G_k$

*Because* ***k*** $\equiv -$***k*** *for each IR only six basis vectors are used:*

All the BV's are complex and their values for IR $\tau_2$ are shown below:

| | $BV_1$ | $BV_2$ | $BV_3$ |
|---|---|---|---|
| 1x | 0 | 0 | 1 |
| 1y | 1 | -1 | 0 |
| 1z | 0 | 0 | 0 |
| 2x | 0 | 0 | 1 |
| 2y | -1 | 1 | 0 |
| 2z | 0 | 0 | 0 |
| 3x | 0 | 0 | -i |
| 3y | i | i | 0 |
| 3z | 0 | 0 | 0 |
| 4x | 0 | 0 | -i |
| 4y | -i | -i | 0 |
| 4z | 0 | 0 | 0 |

| | $BV_4$ | $BV_5$ | $BV_6$ |
|---|---|---|---|
| 1x | -1 | 0 | 0 |
| 1y | 0 | 0 | 0 |
| 1z | 0 | 1 | -1 |
| 2x | -1 | 0 | 0 |
| 2y | 0 | 0 | 0 |
| 2z | 0 | 1 | -1 |
| 3x | -i | 0 | 0 |
| 3y | 0 | 0 | 0 |
| 3z | 0 | i | i |
| 4x | -i | 0 | 0 |
| 4y | 0 | 0 | 0 |
| 4z | 0 | i | i |

*Summary:*

- all BV's are complex
- orientations of magnetic moments (non-zero components) are different for various BV's
- the orientation determines the possible BV's pairs matching: ($BV_1$-$BV_2$), ($BV_3$-$BV_4$), ($BV_5$-$BV_6$)

To produce a real model structure linear combination of BV's is used, with the respective coefficients denoted as: $C_i = A_i + iB_i$ $(i=1,6)$. The general condition for the linear combination to produce a real result leads to a set of linear equations for unknown $A_i, B_i$. The number of unknown variables is $N_v=12$.

After elimination of redundant equations the reduction procedure leads to a set of six equations so $N_e=6$ and for IR $\tau_2$ the final set of equations looks as follows:

$$\begin{aligned} A_1 + A_2 = 0 &\rightarrow A_2 = -A_1 \\ B_1 - B_2 = 0 &\rightarrow B_2 = B_1 \\ A_3 + A_4 = 0 &\rightarrow A_4 = -A_2 \\ B_3 - B_4 = 0 &\rightarrow B_4 = B_3 \\ A_5 + A_6 = 0 &\rightarrow A_6 = -A_5 \\ B_5 - B_6 = 0 &\rightarrow B_6 = B_5 \end{aligned}$$

Translation to the complex $C_i$ coefficients converts the solution to the following form:

$$C_2 = -C_1^* \qquad C_4 = -C_3^* \qquad C_6 = -C_5^*$$

Thus the $C_1$, $C_3$ and $C_5$ coefficients can be chosen as arbitrary values, and can be represented by six arbitrary $A_i, B_i$ values:

$$C_1 = A_1 + i\,B_1 \qquad C_3 = A_3 + i\,B_3 \qquad C_5 = A_5 + i\,B_5$$

For each pair of respective coefficients (pair of respective BV's) there are two free real parameters, which describe the respective magnetic mode uniquely. . Thus fwe have three independent magnetic modes, oriented along *x,y* and *z* directions, which may contribute to the magnetic structure in arbitrary proportions. The respective final solutions for IR $\tau_2$ are presented in Table 2a.

**Table 2a – group 62 – pos. 4(a) – k=(0,0,1/2) - $\tau_2$**

| Site | Position | $\tau_2 - M_x$ | $\tau_2 - M_y$ | $\tau_2 - M_z$ |
|---|---|---|---|---|
| 1 | (0.00, 0.00, 0.00) | [$A_1$,0,0] | [0, $A_2$,0] | [0,0, $A_3$] |
| 2 | (0.00, 0.50, 0.00) | [$A_1$,0,0] | [0,-$A_2$,0] | [0,0, $A_3$] |
| 3 | (0.50, 0.50, 0.50) | [$B_1$,0,0] | [0,-$B_2$,0] | [0,0,-$B_3$] |
| 4 | (0.50, 0.00, 0.50) | [$B_1$,0,0] | [0, $B_2$,0] | [0,0,-$B_3$] |

All modes are collinear and labeled by their respective orientation. The four magnetic sites are divided into two distinct sublattices, controlled by different parameters. Only one mode ($M_y$) is fully compensated i.e. antiferromagnetic.

For IR $\tau_1$ the algebra of the solution is very similar, although the BV's are slightly different. The only difference in the final solutions is a minus sign. The solutions are as follows:

$$C_2 = C_1^* \qquad C_4 = C_3^* \qquad C_6 = C_5^*$$

The calculated magnetic modes for the $\tau_1$ are shown in Table 2b below:

**Table 2b – group 62 – pos. 4(a) – k=(0,0,1/2) - $\tau_1$**

| Site | Position | $\tau_1 - M_x$ | $\tau_1 - M_y$ | $\tau_1 - M_z$ |
|---|---|---|---|---|
| 1 | (0.00, 0.00, 0.00) | [ $A_1$,0,0] | [0,$A_2$,0] | [0,0, $A_3$] |
| 2 | (0.00, 0.50, 0.00) | [-$A_1$,0,0] | [0,$A_2$,0] | [0,0,-$A_3$] |
| 3 | (0.50, 0.50, 0.50) | [-$B_1$,0,0] | [0,$B_2$,0] | [0,0, $B_3$] |
| 4 | (0.50, 0.00, 0.50) | [ $B_1$,0,0] | [0,$B_2$,0] | [0,0,-$B_3$] |

As can be easily noticed all modes are again collinear. For IR $\tau_1$ there are two exactly compensated antiferromagnetic modes $M_x$, $M_z$ , as the magnetic moments are fully compensated for any choice of ($A_1$,$B_1$) and ($A_3$,$B_3$). There was only one such a mode found for $\tau_2$.

As can be seen for both representations the compensation always takes places in the ion pairs (1-2) and (3-4) respectively. In the general case, when all the modes contribute to the structure it may take the form of a noncollinear (canted) ferromagnet or ferrimagnets ($\tau_1$ - $M_y$ and $\tau_2$ – $M_x$, $M_z$) or a fully compensated antiferromagnet ($\tau_1$ – $M_x$, $M_z$ and $\tau_2$ – $M_y$).

The solutions presented above specify the model structure in the so called "zero-cell" i.e. for translation vector equal to zero. The wave vector value (0,0,1/2) tells the rest, i.e. sets the propagation of the solution to an arbitrary cell of the crystal. It can be easily noticed that the solution will take alternating signs in consecutive crystal cells along the z axis, i.e. the magnetic cell will be doubled along the z direction. The solution does not change if the translation vector lies in the (x-y) plane, so the x and y axis period will remain the same.