Example 1:

$k=(0,0,0)$ – space group No. 135 (P 4_2 / m b c) – pos. 4d

Atomic positions:

1: (0.0,0.50,0.25) *2: (0.50,0.0,0.75)*
3: (0.0,0.50,0.75) *4: (0.50,0.0,0.25)*

For that case symmetry analysis shows:

- two 2-d IR's (τ_9 and τ_{10}) and four 1-d IR's ($\tau_3, \tau_4, \tau_5, \tau_6$)
- τ_9, τ_{10} occur two times each in decomposition of magnetic representation.
- all atomic positions form one orbit of the G_k group

For each 2-d IR four (2x2) basis vectors are obtained from MODY:

	IR τ_9				IR τ_{10}			
	BV_1	BV_2	BV_3	BV_4	BV_1	BV_2	BV_3	BV_4
$1x$	1	0	0	i	1	0	0	i
$1y$	0	i	1	0	0	i	1	0
$1z$	0	0	0	0	0	0	0	0
$2x$	0	1	i	0	0	1	i	0
$2y$	$-i$	0	0	-1	$-i$	0	0	-1
$2z$	0	0	0	0	0	0	0	0
$3x$	1	0	0	i	-1	0	0	$-i$
$3y$	0	i	1	0	0	$-i$	-1	0
$3z$	0	0	0	0	0	0	0	0
$4x$	0	1	i	0	0	-1	$-i$	0
$4y$	$-i$	0	0	-1	i	0	0	1.0
$4z$	0	0	0	0	0	0	0	0

Summary:

- all the BV's are complex
- orientation of magnetic moments is in the *(x,y)* plane (zero z-components)
- the non-zero components in BV's indicate how they can be combined to produce real model structures: by matching (BV_1-BV_4) and (BV_2-BV_3)

To produce a real model structure linear combination of BV's is used, with the respective coefficients denoted as: $C_i = A_i + iB_i$ $(i=1,4)$. 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 $N_v=8$. After elimination of redundant equations the reduction procedure leads to a set of four equations so $N_e=4$ and for both IR's the final set of equations looks as follows:

$$\begin{array}{lcl} A_1 + B_4 = 0 & \rightarrow & B_4 = -A_1 \\ B_1 + A_4 = 0 & \rightarrow & A_4 = -B_1 \\ A_2 + B_3 = 0 & \rightarrow & B_3 = -A_2 \\ B_2 + A_3 = 0 & \rightarrow & A_3 = -B_2 \end{array}$$

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

$$C_4 = -i\,C_1^x \qquad C_3 = -i\,C_2^x$$

The obtained result fully confirms the previous conclusion about the BV's matching, showing that pairs BV_1-BV_4 and BV_2-BV_3 can separately produce real model structures i.e. ***magnetic modes*** ($C_2=C_3=0$ or $C_1=C_4=0$ respectively). What's more it can seen that the reality condition leaves the C_1 and C_2 coefficients completely arbitrary:

$$C_1 = A_1 + i\,B_1 = D\,e^{i\phi} \qquad C_2 = A_2 + i\,B_2 = E\,e^{i\psi}$$

Thus for each pair of respective matched BV's there are two free real parameters, which describe the respective magnetic mode uniquely. These parameters are (A_1,B_1) or (D,ϕ) for the (1-4) mode and (A_2,B_2) or (E,ψ) for the (2-3) mode. Thus for each IR two independent magnetic modes are obtained, which can contribute to the magnetic structure in arbitrary proportions. The calculated magnetic modes are shown in Table 1 below.

Table 1 – group 135 – pos. 4(a) – k=(0,0,0)

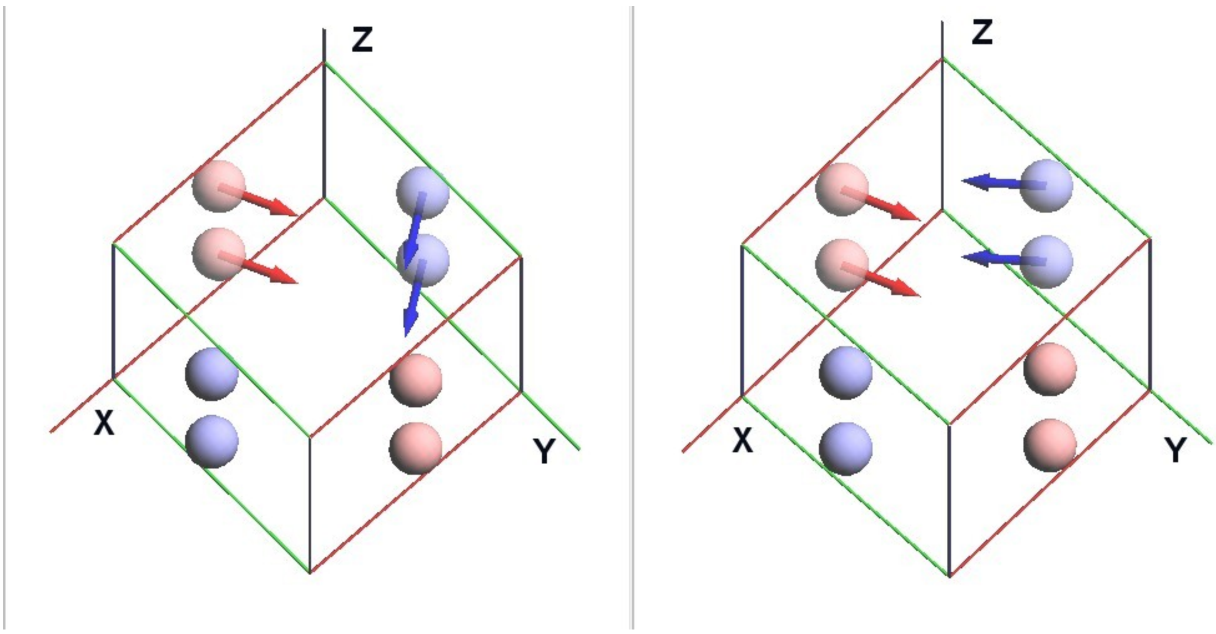
Site	Position	$\tau_9 - M_1$	$\tau_9 - M_2$	$\tau_{10} - M_1$	$\tau_{10} - M_2$
1	(0.00, 0.50, 0.25)	$[A_1, 0,0]$	$[0,B_2,0]$	$[A_1,0,0]$	$[0, B_2,0]$
2	(0.50, 0.00, 0.75)	$[0, B_1,0]$	$[A_2,0,0]$	$[0,-B_1,0]$	$[A_2,0,0]$
3	(0.00, 0.50, 0.75)	$[A_1, 0,0]$	$[0,B_2,0]$	$[-A_1,0,0]$	$[0,-B_2,0]$
4	(0.50, 0.00, 0.25)	$[0, B_1,0]$	$[A_2,0,0]$	$[0, B_1,0]$	$[-A_2,0,0]$

where: A_1=D cos(ϕ), B_1=D sin(ϕ), A_2=E cos(ψ), B_2=E sin(ψ)

From the Table 1 it can be seen that by proper selection of the free parameters various physical models can be obtained. For the general case the magnetic moments on (1,3) and (2,4) sites are different, thus the magnetic sites are divided into two separate subsets (sublattices) governed by different model parameters. Special cases, often welcome by the experimentalists, are the so called constant-moment models, i.e. models with the same magnetic moments on all atomic sites. They can be obtained for individual modes in both representations if $\phi=\pi/4$ and $\psi=\pi/4$ are selected. For such cases $A_1= B_1$ and $A_2= B_2$ and the magnetic moments become equal on all sites for all individual modes.

Another possibility to obtain such a model for a combination of M_1 and M_2 modes is to require that $A_1^2+B_2^2 = A_2^2+B_1^2$, what leads to a magnetic structure with the square of magnetic moments in all sites given by $A_1^2+B_2^2$ and the orientations in the (x,y) plane given by the B_1/A_2 and B_2/A_1 ratios.

The spatial arrangement of magnetic moments for a general combination of M_1 and M_2 modes calculated for the τ_9 representation is shown in the figure below. The magnetic moments may have different values in the red and blue sublattices, and the respective orientation angles in the (x-y) plane are given by B_1/A_2 and B_2/A_1 ratios for the red and blue sites respectively. The left and right figures present configurations for various B_2/A_1 ratio values.



The two modes found for τ_9 representation are noncollinear ferromagnetic configurations. As can be easily noticed from the contents of Table 1 the respective two modes calculated for τ_{10} are fully antiferromagnetic, as the magnetic moments are fully compensated for any choice of (A_1,B_1) and (A_2,B_2).