Example 3:

k=(q_x,q_x,0) – space group No 139 (I4/mmm) – pos. 8f , orbit 1

For that case symmetry analysis shows:

- the 8 atomic positions are split into two orbits of G_k, four sites each
- four 1-d representations τ_1, τ_2, τ_3 and τ_4,
- τ_2 and τ_3 occur two times in the decomposition, while τ_1 and τ_4 occur only once for the $(q_x,q_x,0)$ wave vector.

Atomic positions:

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

*For IR τ_3 four basis vectors are calculated from MODY (for **k** and –**k**):*

IR τ_3 (+*k*)

	BV_1	BV_2
1x	1	0
1y	1	0
1z	0	1
2x	-1	0
2y	-1	0
2z	0	1
3x	a	0
3y	a	0
3z	0	a
4x	-a	0
4y	-a	0
4z	0	-a

IR τ_3 (-*k*)

	BV_3	BV_4
1x	a^*	0
1y	a^*	0
1z	0	a^*
2x	$-a^*$	0
2y	$-a^*$	0
2z	0	a^*
3x	b^*	0
3y	b^*	0
3z	0	b^*
4x	$-b^*$	0
4y	$-b^*$	0
4z	0	b*

the additional parameters ***a,b*** are given by:

$$a = e^{i2\pi q_x} = e^{i2\alpha} \qquad b = e^{i4\pi q_x} = e^{i4\alpha}$$

It can be seen that for both $+k$ and $-k$ for one of the BV's the magnetic moments lie in the (x,y) plane, while for the other one in the z direction.

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 IR τ_3 the final set of equations looks as follows:

$$\begin{aligned} &B_1 + gA_3 - hB_3 = 0 \\ &gA_1 + hB_1 + A_3 + pB_3 = 0 \\ &B_2 + gA_4 - hB_4 = 0 \\ &gA_2 + hB_2 + A_4 + pB_4 = 0 \end{aligned}$$

where g,h,p are constants dependent on the $\alpha=\pi q_x$ value.

It can be seen that A_3, B_3 couple only to A_1, B_1 and A_4, B_4 couple only to A_2, B_2. This is again a direct indication that the system of equation separates into two pairs of equations, describing two pairs of matching basis vectors. Each pair of equations can be solved separately and after converting the relations to the C_i coefficients the solution looks as follows:

$$C_3 = aC_1^* \qquad C_4 = aC_2^*$$

Again it can be seen that the reality condition leaves the C_1 and C_2 with arbitrary values. It is convenient to express these coefficients by four real parameters, namely their amplitudes and phases:

$$\begin{aligned} C_1 &= C\exp(i\phi_1) \quad & C_3 &= C\exp(i2\alpha)\exp(-i\phi_1) \\ C_2 &= D\exp(i\phi_2) \quad & C_4 &= D\exp(i2\alpha)\exp(-i\phi_2) \end{aligned}$$

Thus it turns out that the solutions allows four real free parametersand the parameters can be represented as two amplitudes and two free phases describing the model structure. Using such coefficients for calculation of the linear combination of BV's leads to the final solution describing the model structure.

The results of the calculation can be found in the first part of Table 1 below. Thus IR τ_3 allows two independent "magnetic waves" with arbitrary amplitudes and phases in the symmetry adapted magnetic structure model for Orbit 1.

Table 1 – group 139 – k=(q_x,q_x,0) – pos. 8f – orbit 1+2

Orb.1	Position	$\tau_3 - M_1$	$\tau_3 - M_2$
1	(0.25, 0.25, 0.25)	[C,C,0] cos(kt+α+ϕ_1)	[0,0, D] cos(kt+α+ϕ_2)
2	(0.25, 0.25, 0.75)	[-C,-C,0] cos(kt+α+ϕ_1)	[0,0,D] cos(kt+α+ϕ_2)
3	(0.75, 0.75, 0.75)	[C,C,0] cos(kt+3α+ϕ_1)	[0,0, D] cos(kt+3α+ϕ_2)
4	(0.75, 0.75, 0.25)	[-C,-C,0] cos(kt+3α+ϕ_1)	[0,0, D] cos(kt+3α+ϕ_2)
Orb.2			
5	(0.25, 0.75, 0.75)	[E,-E,0] cos(kt+2α+ϕ_3)	[0,0,F] cos(kt+2α+ϕ_4)
6	(0.75, 0.25, 0.75)	[-E,E,0] cos(kt+2α+ϕ_3)	[0,0,F] cos(kt+2α+ϕ_4)
7	(0.75, 0.25, 0.25)	[E,-E,0] cos(kt+2α+ϕ_3)	[0,0, F] cos(kt+2α+ϕ_4)
8	(0.25, 0.75, 0.25)	[-E,E,0] cos(kt+2α+ϕ_3)	[0,0,F] cos(kt+2α+ϕ_4)

After repeating the calculation for the second orbit and construction of the linear combination of BV's with the obtained C_m coefficients the complete magnetic structure model is obtained. Short summary of the obtained magnetic structure model is shown in the Table 1.

Now in the final result we have two independent orbits, with two independent modes on each orbit. Thus for the 8(f) positions there are eight free parameters: four amplitudes C,D,E,F and four free phases ϕ_1, ϕ_2, ϕ_3, ϕ_4. The resulting structure contains two flat cycloids with magnetic moment turning in the plane perpendicular to [1,-1,0] direction for the first orbit and in the plane perpendicular to [1,1,0] direction for the second orbit (spiral configuration). Again the tips of the magnetic moment vectors in general walk along a Lissajous curve, the shape of which depends on the amplitudes C,D,E,F and the phase differences $\phi_2-\phi_1$, $\phi_4-\phi_3$.

The phase differences between the individual ions result from their location in space. The phase of the magnetic wave on each ion is determined by the phase at the origin of the given unit cell and the additional phase correction result from the position of the ion in the unit cell (various $\boldsymbol{k}\cdot\boldsymbol{r}_n$ values). The phase corrections make the individual ions form a complete sinusoidal wave propagating across the unit cell. For the structure shown in the table the α–dependent extra phase correction is pinned to zero for $\boldsymbol{k}\cdot\boldsymbol{r}_n = 0$. In principle the phase calibration are completely independent on both orbits, so it only a matter of convenience to chose the phases consistently for both orbits and with reference to the cell origin. One phase relation that holds idependently of the phase calibration is the phase difference between origins of two neigbouring unit cells.

Figure 1 below present the spatial arrangement of magnetic moments in the symmetry-adapted structure model consistent with the τ_3 representation. Orbits 1 and 2 are denoted by green and red sites respectively. It can be noticed that all ions in Orbit 2 are in the same phase, while two pairs of atoms in Orbit 1 definitely exhibit phase difference, manifested by the additional turning angle of the cycloid.