

Description of multi-k magnetic structures from powder neutron diffraction data

Ovi Garlea
Neutron Scattering Division,
Oak Ridge National Laboratory



ORNL is managed by UT-Battelle, LLC for the US Department of Energy



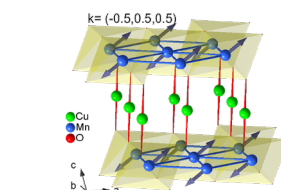
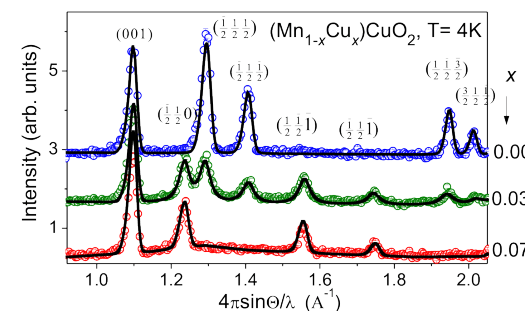
U.S. DEPARTMENT OF
ENERGY

Multi-k magnetic structure situations

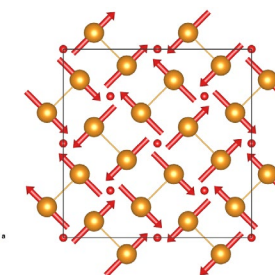
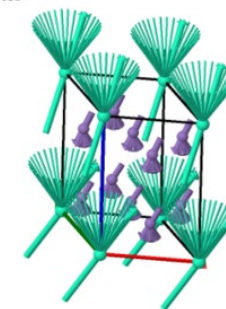
- Inhomogeneous sample or multiple magnetic ground states with similar energies
 - two or more non-equivalent k vectors that can be treated as multiple magnetic phases
- Structures where different moment components are described by different k -vectors (canted helical structures)
 - non-equivalent k vectors that can be looked as two magnetic phases
- Structures with multi- k of the same “star” (Hard to distinguish from single- k structures)
 - distinct k -vectors applies to different magnetic sites

D. Khalyavin

- multiple k -vectors act concomitantly on all sites (Skyrmion lattices)

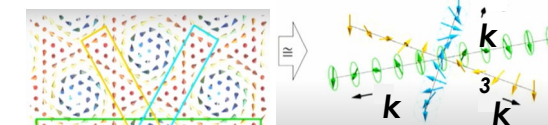


DyMn_6Ge_6
 $k_1 = (0, 0, 0)$,
 $k_2 = (0, 0, 0.165)$

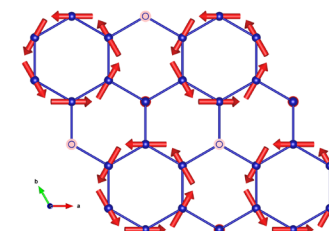


2- k - order in $\text{BaNd}_2\text{ZnO}_5$

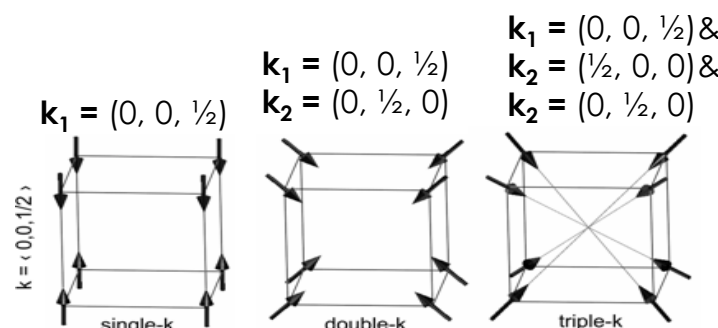
Skyrmion lattices



3- k order in Gd_2PdSi_3
 (D. Khalyavin)

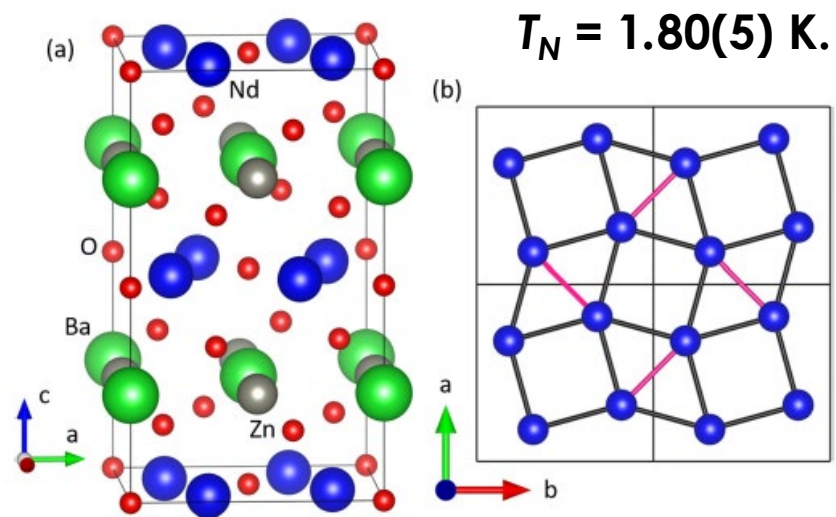


3- k order in $\text{Na}_2\text{Co}_2\text{TeO}_6$



2k- order in the Shastry-Sutherland lattice of $\text{BaNd}_2\text{ZnO}_5$

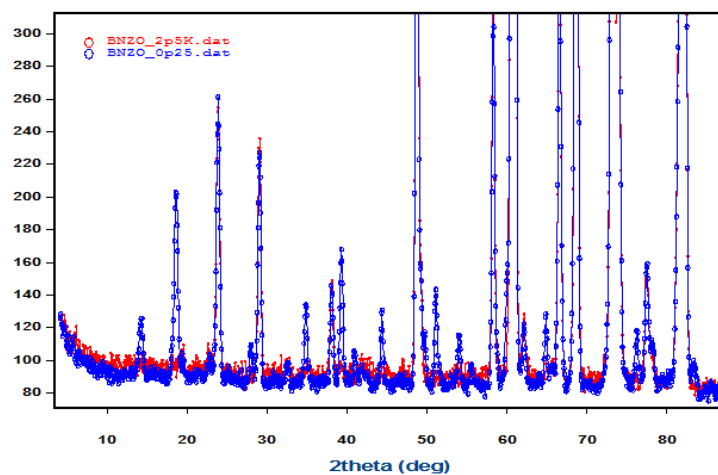
Y. Ishii et al, [10.1103/PhysRevMaterials.5.064418](https://doi.org/10.1103/PhysRevMaterials.5.064418)



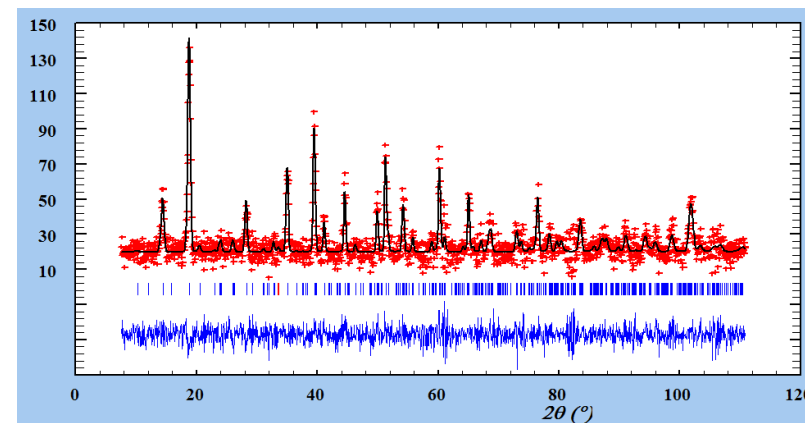
$I4/mcm$ (#140)

Atom	x	y	z	usio
Ba	0	0	0.25	0.5(1)
Nd1	0.1736(2)	0.6736(2)	0	0.11(6)
Zn	0	0.5	0.25	0.33(9)
O1	0	0	0	0.3(1)
O2	0.3547(1)	0.8547(1)	0.1312(1)	0.66(6)

data measured at 250mK and 2.5K :

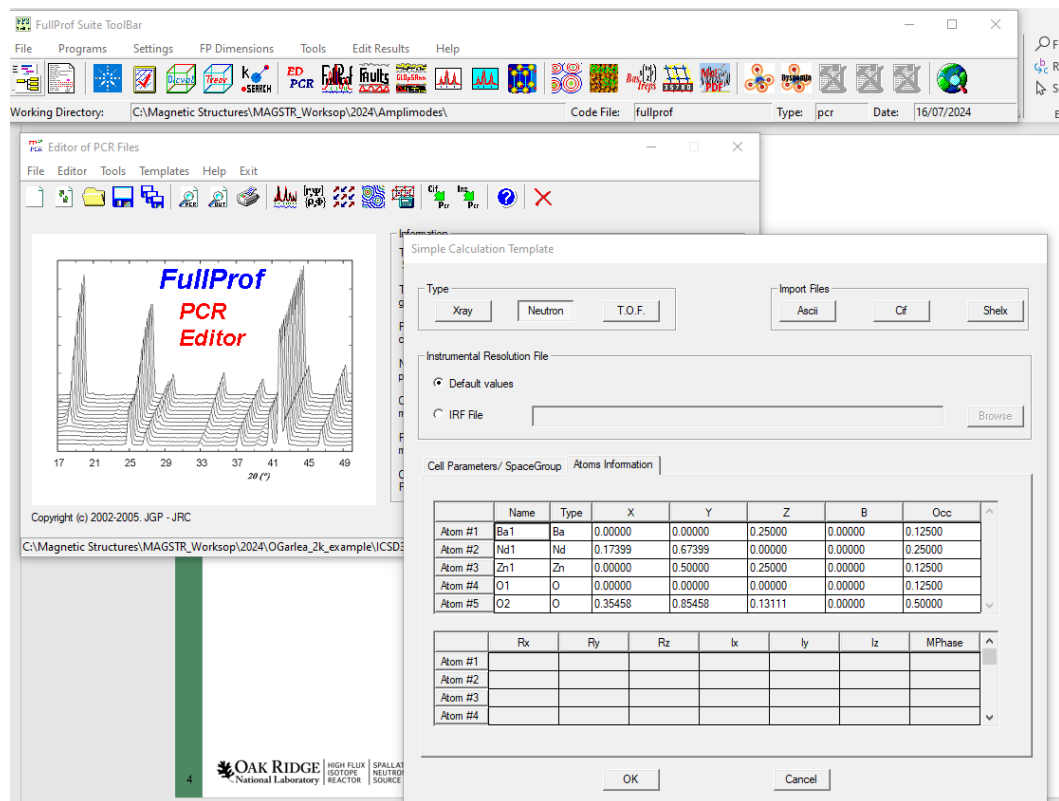


difference data 250mK - 2.5K



Use the steps given in previous examples to create a crystal model for fitting the nuclear peaks

load the model from [ICSD35906.cif](#), and use the “[hb2a_2p41A_resolution.irf](#)” and data file “[BNZO_0p25.dat](#)” (in X-Y-Err format / Ins 10)

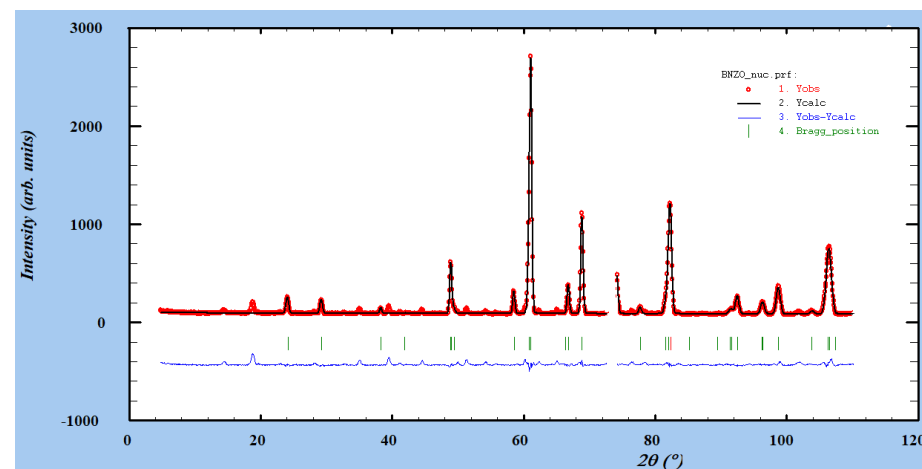


! Excluded regions (LowT HighT)

72.50 74.00

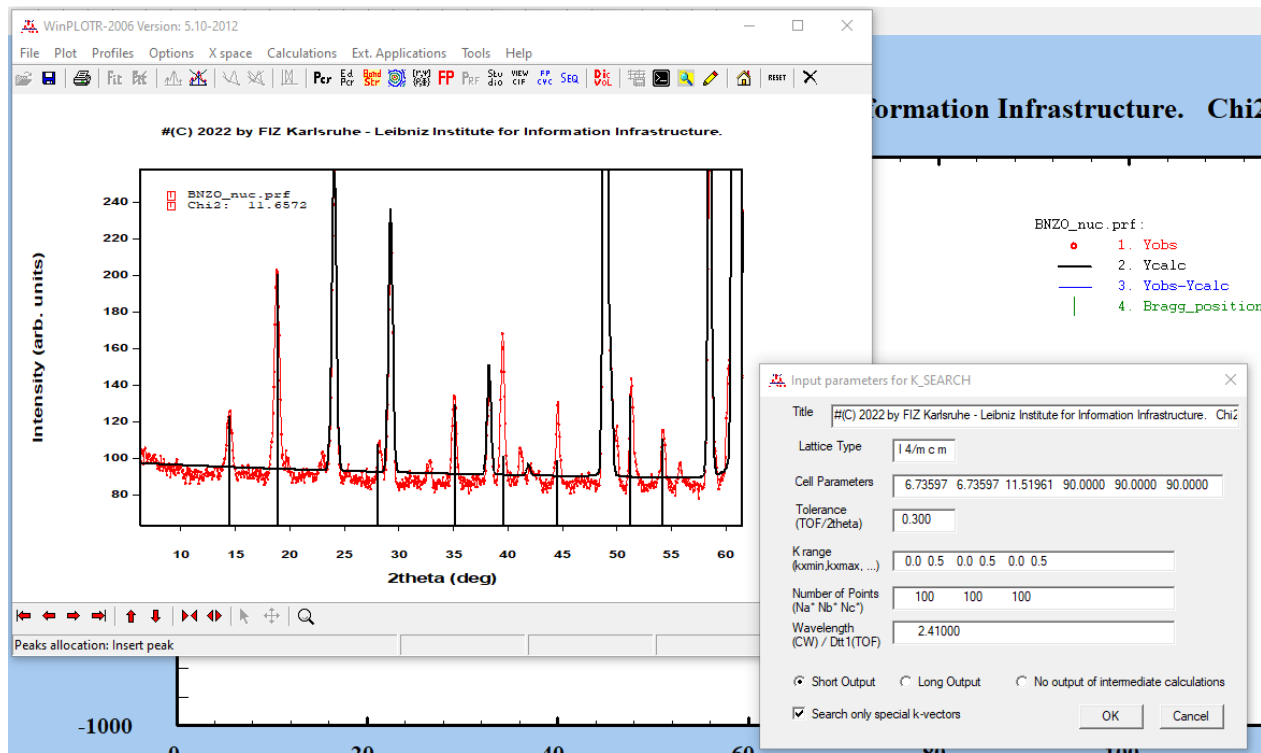
110.00 150.00

Aluminum peaks due to sample holder are ignored in this example



The resulted PCR file for fitting the nuclear contribution in: [BNZO_nuc.pcr](#)

Use the `BNZO_nuc.prf` to select the magnetic peaks and find the k-vector using the k-search program



```

C:\WINDOWS\SYSTEM32\cmd.exe
=> Writing partial results ...

=> Testing 90 internal k-vectors
Solution: 1 k =( 0.5000 0.5000 0.0000) R-F: 2.0149
Solution: 2 k =( 0.5000 0.2500 0.2500) R-F: 2.4468
Solution: 3 k =( 0.2500 0.5000 0.2500) R-F: 2.4468
=> Special k-vector solutions found!

=> List of the best incommensurate 10 solutions for 8 satellites

      Kx      Ky      Kz      R-factor
0.500000    0.500000    0.000000    2.014893
0.500000    0.250000    0.250000    2.446817
0.250000    0.500000    0.250000    2.446817

=> The best commensurate solution is the special kvector ks =( 0.5000 0.5000 0.0000)
=> The corresponding R-factor is:      2.0149 to be compared with incommensurate R-factors

=> Powder diffraction may give wrong results even if the R-factors for the solutions are "good"
    The best way to verify the solutions is to perform a full profile fitting and look for mismatches

      Total CPU-Time

      CPU-seconds:      0.02
      CPU-minutes:      0.00
      CPU-hours :      0.00

=> Press <enter> to finish
  
```

The determined propagation vector is $k = (\frac{1}{2}, \frac{1}{2}, 0)$

Explore the possible magnetic models compatible a single $k = (\frac{1}{2}, \frac{1}{2}, 0)$, using the MAXMAGN in BCS

MAXMAGN: Maximal magnetic space groups for a given a propagation vector and resulting magnetic structural models

MAXMAGN: Maximal magnetic space groups for a given a propagation vector and resulting magnetic structural models

MAXMAGN provides the possible magnetic space groups that can be assigned to a 1-k commensurate magnetic phase assuming that the magnetic symmetry is a maximal one. The space group of the paramagnetic phase (parent group) and the observed propagation vector are required as input. Optionally, the parent paramagnetic structure can be introduced (by hand or by a cif file). In this latter case the program provides the constraints for the different possible symmetries and cif-like files can be produced. These files permit the different alternative models to be analyzed, refined, shown graphically.

☒ Structure data of the paramagnetic phase will be included

☐ Non-conventional setting

Please, enter the label of the space group of the paramagnetic phase (parent group)

choose it 140

Please, enter the propagation vector k:

k_x 0.5 k_y 0.5 k_z 0

Submit

2	Nd1_1 Nd 0.08700 0.33700 0.00000	(x,x+1/4,0 $m_x, -m_x, 0$) (-x,-x+1/4,0 $m_x, -m_x, 0$) (x+1/4,x,1/2 $m_x, -m_x, 0$) (-x+1/4,-x,1/2 $m_x, -m_x, 0$) (x,x+3/4,0 $-m_x, m_x, 0$) (-x,-x+3/4,0 $-m_x, m_x, 0$) (x+1/4,x+1/2,1/2 $-m_x, m_x, 0$) (-x+1/4,-x+1/2,1/2 $-m_x, m_x, 0$) (x+1/2,x+1/4,0 $-m_x, m_x, 0$) (-x+1/2,-x+1/4,0 $-m_x, m_x, 0$) (x+3/4,x,1/2 $-m_x, m_x, 0$) (-x+3/4,-x,1/2 $-m_x, m_x, 0$) (x+1/2,x+3/4,0 $m_x, -m_x, 0$) (-x+1/2,-x+3/4,0 $m_x, -m_x, 0$) (x+3/4,x+1/2,1/2 $m_x, -m_x, 0$) (-x+3/4,-x+1/2,1/2 $m_x, -m_x, 0$)	16	$(M_x, -M_x, 0)$	$M_x = 2$
	Nd1_2 Nd 0.16301 0.08700 0.00000	(-x+1/4,x,0 $m_x, -m_x, 0$) (x+1/4,-x,0 $m_x, -m_x, 0$) (-x,x+1/4,1/2 $m_x, -m_x, 0$) (x,-x+1/4,1/2 $m_x, -m_x, 0$) (-x+1/4,x+1/2,0 $-m_x, m_x, 0$) (x+1/4,-x+1/2,0 $-m_x, m_x, 0$) (-x,x+3/4,1/2 $-m_x, m_x, 0$) (x,-x+3/4,1/2 $-m_x, m_x, 0$) (-x+3/4,x,0 $-m_x, m_x, 0$) (x+3/4,-x,0 $-m_x, m_x, 0$) (-x+1/2,x+1/4,1/2 $-m_x, m_x, 0$) (x+1/2,-x+1/4,1/2 $-m_x, m_x, 0$) (-x+3/4,x+1/2,0 $m_x, -m_x, 0$) (x+3/4,-x+1/2,0 $m_x, -m_x, 0$) (-x+1/2,x+3/4,1/2 $m_x, -m_x, 0$) (x+1/2,-x+3/4,1/2 $m_x, -m_x, 0$)	16	$(M_x, -M_x, 0)$	$M_x = 2$

Save the MCIF file corresponding to the MSG

C_{4mca} (#64.480)

Transform to standard: $1/2a-1/2b,c,-1/2a-1/2b;1/4,0,0$

Load structure from ICSD35906.cif

Maximal subgroups which allow non-zero magnetic moments for at least one atom are coloured

N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	C_{4cca} (#68.520) Go to a subgroup	$\begin{pmatrix} 0 & -1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
2	C_{4mma} (#67.510) Go to a subgroup	$\begin{pmatrix} 0 & -1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
3	C_{4ccm} (#66.500) Go to a subgroup	$\begin{pmatrix} 0 & -1 & 1 & 1/4 \\ 0 & 1 & 1 & 1/4 \\ -1 & 0 & 0 & 1/4 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
4	C_{4mmm} (#65.490) Go to a subgroup	$\begin{pmatrix} 0 & -1 & 1 & 1/2 \\ 0 & 1 & 1 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
5	C_{4mca} (#64.480) Go to a subgroup	$\begin{pmatrix} 1 & 0 & -1 & 1/2 \\ -1 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
6	C_{4mca} (#64.480) Go to a subgroup	$\begin{pmatrix} 0 & -1 & 1 & 1/2 \\ 0 & 1 & 1 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
7	C_{4mcm} (#63.468) Go to a subgroup	$\begin{pmatrix} 0 & -1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show
8	C_{4mcm} (#63.468) Go to a subgroup	$\begin{pmatrix} 1 & 0 & -1 & 1/4 \\ -1 & 0 & -1 & 7/4 \\ 0 & 1 & 0 & 1/4 \end{pmatrix}$ Alternatives (domain-related)	Show	Systematic absences MAGNEXT Tensor properties MTENSOR	Show

Create a PCR from MCIF using the FullProf ToolBar

```

=> Shubnikov Number: 0
=> BNS Number: 64.480
=> OG Number:
=> BNS Symbol: C_Amca
=> OG Symbol:
=> UNIFIED Symbol:
=> Type of Magnetic group: 4
=> Parent group number: 140
=> Parent group Symbol: I 4/m c m
=> Magnetic point group Symbol:
=> Laue Class for Cell constr.:
=> Transformation to parent: a,b,c;0,0,0
=> Transformation from parent: 2a,2b,c;0,0,0
=> Transformation to standard: 1/2a-1/2b,c,-1/2a-1/2b;1/4,0,0
=> Transformation from standard:
=> Crystal system:
=> Lattice type:
=> Lattice type Symbol:
=> Number of centring vectors: 3
=> Number of anti-translations: 4
=> Number of reduced set of S.O.: 8
=> General Multiplicity: 64
=> Centred: 0
=> Centre at: (0,1/4,0)
=> Centrosymmetry: Centric (-1 not at origin)
=> Generators (exc. -1&L): 0
=> Centring vectors: 3
=> Latt( 1): (1/2,1/2,0) => Latt( 2): (3/4,1/4,1/2)
  
```

```

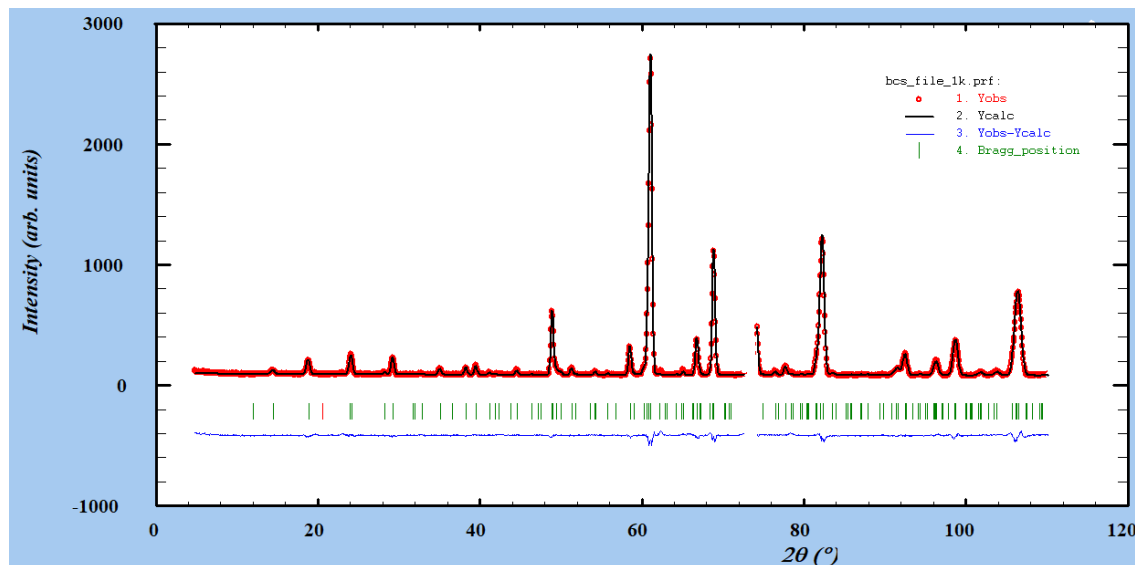
! Data for PHASE number: 1 ==> Current R_Bragg for Pattern# 1: 999.00
!
! Nuclear and Magnetic Structure of: bcs_file_1k VARY mxmymz
!
! Nat Dis Ang Pr1 Pr2 Pr3 Jbt Inf Isy Str Furth ATZ Nvk Npr More
! 7 0 0 0.0 0.0 1.0 10 0 2 0 0 0.000 0 7 0
!
! C_Amca number:64.480 <-Magnetic Space group symbol (BNS/UNI symbol & number)
! Transform to standard: 1/2a-1/2b,c,-1/2a-1/2b;1/4,0,0
! Parent Space Group: I4/mcm IT_number: 140
! Transform from Parent: 2a,2b,c;0,0,0
! Nsym Cen N_Clat N_Ant
! 8 0 3 4
!
! Centring vectors
! 0.50000 0.50000 0.00000
! 0.75000 0.25000 0.50000
! 0.25000 0.75000 0.50000
!
! Anti-Centring vectors
! 0.00000 0.50000 0.00000
! 0.50000 0.00000 0.00000
! 0.25000 0.25000 0.50000
! 0.75000 0.75000 0.50000
!
! Symmetry operators
! 1 x,y,z,+1
! 2 -x,-y,-z,-1
! 3 -x,-y,z,+1
! 4 x,y,-z,-1
! 5 y,x,z+1/2,+1
! 6 -y+1/4,-x+1/4,-z,+1
! 7 -y+1/4,-x+1/4,z,-1
! 8 y,x,-z+1/2,-1
!
! Atom Typ Mag Vek X Y Z Biso Occ N_type Spc /Line below:Codes
! Rx Ry Rz Ix Iy Iz MagPh / Line below:Codes
! Ba1 Ba beta11 beta22 beta33 beta12 beta13 beta23 / Line below:Codes
! 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! Nd1_1 JND3 1 0 0.08700 0.33700 0.00000 0.00000 0.25000 1 0 #
! 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! 2.00000 -2.00000 0.00000 0.00000 0.00000 0.00000 0.00000 <-MagPar
! 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! Nd1_2 JND3 1 0 0.16301 0.08700 0.00000 0.00000 0.25000 1 0 #
! 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! 2.00000 -2.00000 0.00000 0.00000 0.00000 0.00000 0.00000 <-MagPar
! 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! Zn1 Zn 1 0 0.00000 0.25000 0.25000 0.00000 0.25000 0 0 #
! 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! O1 O 1 0 0.00000 0.00000 0.00000 0.00000 0.25000 0 0 #
! 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! O2_1 O 1 0 0.17729 0.42729 0.13111 0.00000 0.50000 0 0 #
! 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! O2_2 O 1 0 0.07271 0.17729 0.13111 0.00000 0.50000 0 0 #
! 0.00 0.00 0.00 0.00 0.00 0.00 0.00
  
```

Modify the created PCR with the correct instrument parameter information from the nuclear_PCR file.

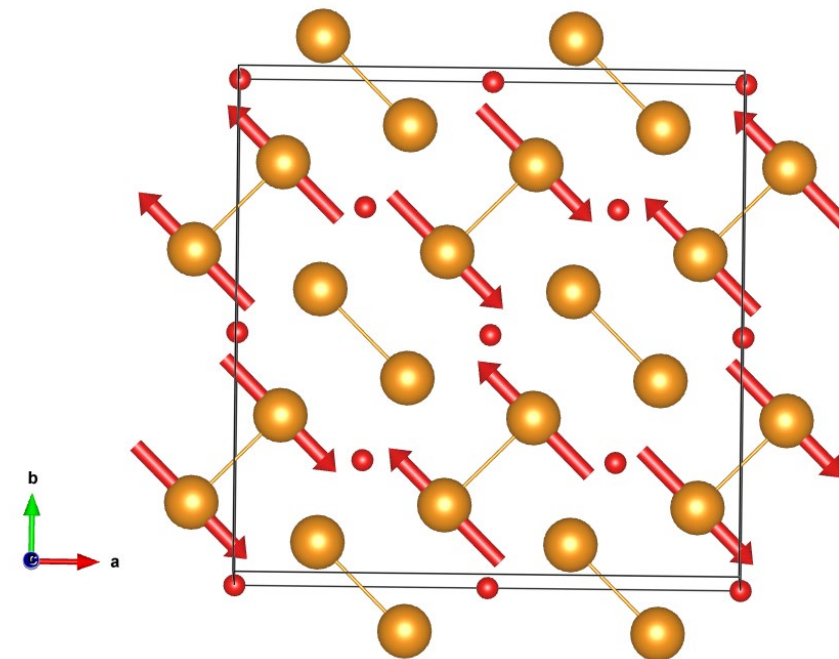
Make sure to maintain the new supercell
(2a, 2a, c)

!	a	b	c
	13.4723	13.4723	11.5195

Perform the refinement on the BNZO_0p25.dat data



!Atom	Typ	Mag	Vek	X	Y	Z	Biso	Occ	N_type	Spc/Fftype	/l
!	Rx	Ry		Rz	Ix	Iy	Iz	MagPh	/ Line	below:Codes	
!	beta11	beta22		beta33	beta12	beta13	beta23				
Ba1	Ba	1	0	0.00000	0.00000	0.25000	0.00000	0.25000	0	0	#
				0.00	0.00	0.00	0.00	0.00			
Nd1_1	JND3	1	0	0.08700	0.33700	0.00000	0.00000	0.25000	1	0	#
				0.00	0.00	0.00	0.00	0.00			
	1.75624	-1.75624		0.00000	0.00000	0.00000	0.00000	0.00000	<-MagPar		
	-31.00	31.00		0.00	0.00	0.00	0.00	0.00			
Nd1_2	JND3	1	0	0.16301	0.08700	0.00000	0.00000	0.25000	1	0	#
				0.00	0.00	0.00	0.00	0.00			
	-0.12001	0.12001		0.00000	0.00000	0.00000	0.00000	0.00000	<-MagPar		
	-21.00	21.00		0.00	0.00	0.00	0.00	0.00			
Zn1	Zn	1	0	0.00000	0.25000	0.25000	0.00000	0.25000	0	0	#
				0.00	0.00	0.00	0.00	0.00			
O1	O	1	0	0.00000	0.00000	0.00000	0.00000	0.25000	0	0	#



The single k-model consists of two Nd sites with very different moments. One Nd moment is nearly zero, which can't be explained considering the same crystallographic environment

Explore the possible magnetic models compatible a double-k , ($\frac{1}{2}$, $\frac{1}{2}$, 0) and ($\frac{1}{2}$, $-\frac{1}{2}$, 0) using the k-SUBGROUPSMAG

Bilbao Crystallographic Server → k-Subgroupsmag

Help

k-Subgroupsmag: Magnetic subgroups compatible with some given propagation vector(s) or a supercell.

k-Subgroupsmag

The program *k-Subgroupsmag* provides the possible magnetic subgroups of the space group of a paramagnetic phase (gray group) which are possible for a magnetic ordering having a known propagation vector. The program provides the set of magnetic subgroups or a graph showing the subgroup-tree (grouped into conjugacy classes). In both cases, more information about the classes or subgroups can be obtained.

Other alternatives for the input of the program:

- An alternative parent (non gray) magnetic group can be chosen.
- Instead of the whole set of subgroups, the output can be limited to subgroups having a chosen common subgroup of lowest symmetry, common point group of lowest symmetry or groups which

Enter the serial number of the space group of the parent paramagnetic phase:

choose it 140

[Choose an alternative magnetic group](#)

Introduce the magnetic wave vector(s)

(Give the components of the wave vectors in a fractional form, n/m)

k_{1x} 0.5 k_{1y} 0.5 k_{1z} 0

k_{2x} 0.5 k_{2y} -0.5 k_{2z} 0

k_{3x} k_{3y} k_{3z}

[Show the independent vectors of the star](#)

☐ Choose the whole star of the propagation vector

☐ Optionally give also non-magnetic modulation wave-vectors

Parent space group: *I4/mcm* (No. 140)

Lattice parameters (Angstroms and degrees): a=6.73622, b=6.73622, c=11.51950, alpha=90., beta=90., gamma=90.

Atoms: Please select the magnetic ones

N	Atom name	Atom type	Wyckoff Position	Coordinates	Magnetic?
1	Ba1	Ba	4a	0.00000 0.00000 0.25000	☐
2	Nd1	Nd	8h	0.17399 0.67399 0.00000	☒
3	Zn1	Zn	4b	0.00000 0.50000 0.25000	☐
4	O1	O	4c	0.00000 0.00000 0.00000	☐
5	O2	O	16i	0.35458 0.85458 0.13111	☐

Load crystallographic information from [ICSD35906.cif](#)

Select the MSG
*P*_C4/ncc (#130.433)

Subgroups of the paramagnetic space group :
Lowest magnetic space group to consider:
Magnetic propagation wave-vectors

*I4/mcm*1' (N. 140)
*P*1 (N. 1.1)
(0.5,0.5,0),(0.5,-0.5,0)

List of subgroups that fulfill the given conditions

[Get the subgroup-graph](#)

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps	Magnetic structure models (MAGMODELIZE)
1	<i>P</i> _C 4 ₂ / <i>nmc</i> (No. 137.517)	$\begin{pmatrix} 1 & -1 & 0 & 1/2 \\ 1 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=4x1	Conjugacy Class	Get irreps	☐
2	<i>P</i> _C 4 ₂ / <i>mbc</i> (No. 135.493)	$\begin{pmatrix} 1 & -1 & 0 & 1/2 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=4x1	Conjugacy Class	Get irreps	☐
3	<i>P</i> _C 4 ₂ / <i>nbc</i> (No. 133.469)	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=4x1	Conjugacy Class	Get irreps	☐
4	<i>P</i> _C 4 ₂ / <i>mmc</i> (No. 131.445)	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=4x1	Conjugacy Class	Get irreps	☐
5	<i>P</i> _C 4/ <i>ncc</i> (No. 130.433)	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=4x1	Conjugacy Class	Get irreps	☒
6	<i>P</i> _C 4/ <i>mnc</i> (No. 128.409)	$\begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=4x1	Conjugacy Class	Get irreps	☐
7	<i>P</i> _C 4/ <i>inn</i> (No. 126.385)	$\begin{pmatrix} 1 & -1 & 0 & 1/2 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	4=4x1	Conjugacy Class	Get irreps	☐
8	<i>P</i> _C 4/ <i>mcc</i> (No. 124.361)	$\begin{pmatrix} 1 & -1 & 0 & 1/2 \\ 1 & 1 & 0 & 1/2 \end{pmatrix}$	4=4x1	Conjugacy Class	Get irreps	☐

Select the MSG P_C4/ncc (#130.433)

Atomic positions, Wyckoff positions and Magnetic Moments

N	Atom	New WP	Multiplicity	Magnetic moment	Values of M _x , M _y , M _z
1	Ba1_1 Ba 0.00000 0.00000 0.25000	(0,0,1/4 0,0,m _z) (0,0,3/4 0,0,-m _z) (0,1/2,1/4 0,0,-m _z) (0,1/2,3/4 0,0,m _z) (1/2,0,1/4 0,0,-m _z) (1/2,0,3/4 0,0,m _z) (1/2,1/2,1/4 0,0,m _z) (1/2,1/2,3/4 0,0,-m _z)	8	-	-
	Ba1_2 Ba 0.25000 0.25000 0.75000	(1/4,1/4,3/4 0,0,0) (1/4,1/4,1/4 0,0,0) (1/4,3/4,3/4 0,0,0) (1/4,3/4,1/4 0,0,0) (3/4,1/4,3/4 0,0,0) (3/4,1/4,1/4 0,0,0) (3/4,3/4,3/4 0,0,0) (3/4,3/4,1/4 0,0,0)	8	-	-
2	Nd1 Nd 0.08700 0.33700 0.00000	(x,x+1/4,0 m _x ,m _y ,0) (-x,-x+1/4,0 m _x ,m _y ,0) (-x+1/4,x,0 m _y ,m _x ,0) (x+1/4,-x,0 m _y ,m _x ,0) (x+1/4,x,1/2 -m _y ,m _x ,0) (-x+1/4,-x,1/2 -m _y ,m _x ,0) (-x,x+1/4,1/2 m _x ,m _y ,0) (x,-x+1/4,1/2 m _x ,m _y ,0) (x,x+3/4,0 -m _x ,m _y ,0) (-x,-x+3/4,0 -m _x ,m _y ,0) (-x+1/4,x+1/2,0 -m _y ,m _x ,0) (x+1/4,-x+1/2,0 -m _y ,m _x ,0) (x+1/4,x+1/2,1/2 m _x ,m _y ,0) (-x+1/4,-x+1/2,1/2 m _x ,m _y ,0) (-x,x+3/4,1/2 -m _x ,m _y ,0) (x,-x+3/4,1/2 -m _x ,m _y ,0) (x+1/2,x+1/4,0 -m _x ,m _y ,0) (-x+1/2,-x+1/4,0 -m _x ,m _y ,0) (-x+3/4,x,0 -m _y ,m _x ,0) (x+3/4,-x,0 -m _y ,m _x ,0) (x+3/4,x,1/2 m _x ,m _y ,0) (-x+3/4,-x,1/2 m _x ,m _y ,0) (-x+1/2,x+1/4,1/2 -m _x ,m _y ,0) (x+1/2,-x+1/4,1/2 -m _x ,m _y ,0) (x+1/2,x+3/4,0 m _x ,m _y ,0) (-x+1/2,-x+3/4,0 m _x ,m _y ,0) (-x+3/4,x+1/2,0 -m _y ,m _x ,0) (x+3/4,-x+1/2,0 -m _y ,m _x ,0) (x+3/4,x+1/2,1/2 m _x ,m _y ,0) (-x+3/4,-x+1/2,1/2 m _x ,m _y ,0) (-x+1/2,x+3/4,1/2 -m _x ,m _y ,0) (x+1/2,-x+3/4,1/2 -m _x ,m _y ,0)	32	(M _x ,M _y ,0)	M _x = 2 M _y = 2

Modify the created PCR with the correct instrument parameter information from the nuclear_PCR file. The new supercell is the same as for the 1k structure (2a, 2a, c)

Create a PCR from MCIF using the FullProf ToolBar

```

C:\WINDOWS\SYSTEM32\cmd.exe
> Shubnikov Number: 0
> BNS Number: 130.433
> OG Number:
> BNS Symbol: P_C4/ncc
> OG Symbol:
> UNIFIED Symbol:
> Type of Magnetic group: 4
> Parent group number: 140
> Parent group Symbol: I 4/m c m
> Magnetic point group Symbol:
> Leave Class for Cell constr.:
> Transformation to parent: a,b,c;0,0,0
> Transformation from parent: 2a,2b,c;0,0,0
> Transformation to standard: 1/2a+1/2b,-1/2a+1/2b,c;0,1/4,0
> Transformation from standard:
> Crystal system:
> Lattice type:
> Lattice type Symbol:
> Number of centring vectors: 1
> Number of anti-translations: 2
> Number of reduced set of S.O.: 16
> General Multiplicity: 64
> Centred: 0
> Centre at: (0,0,1/4)
> Centrosymmetry: Centric (-1 not at origin)
> Generators (exc. -1&L): 0
> Centring vectors: 1
> Latt(1): (1/2,1/2,0)
  
```

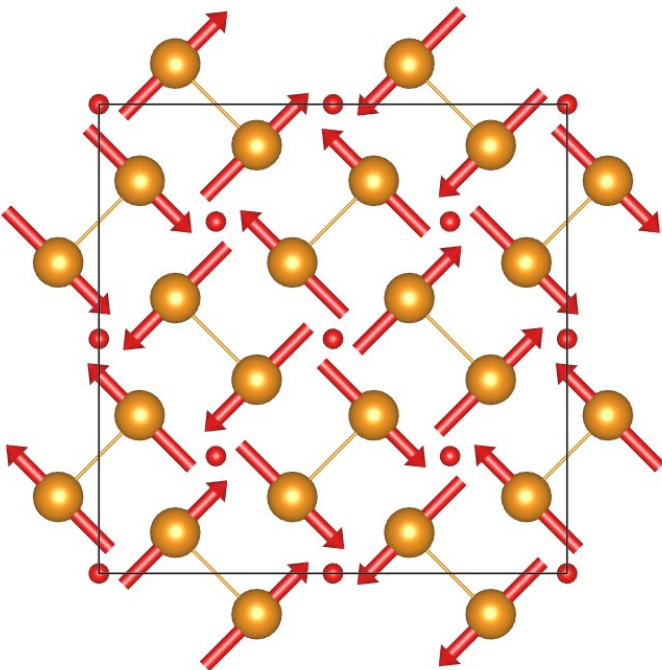
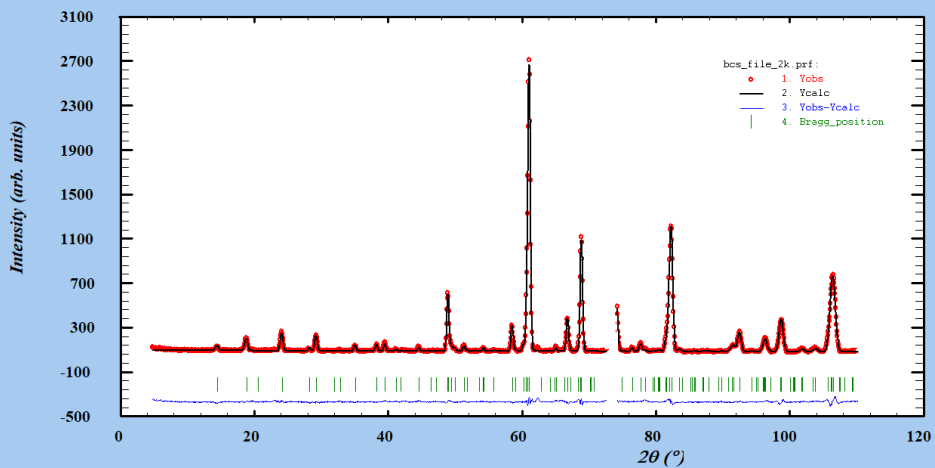
```

bcs_file_2k.pcr - Notepad
File Edit Format View Help
! Zero Code SyCos Code SySin Code Lambda Code MORE ->Patt# 1
0.00 0.00 0.00 0.00 0.00 0.00000 0.00 0
! Data for PHASE number: 1 ==> Current R_Bragg for Pattern# 1: 999.00
!-----
Nuclear and Magnetic Structure of: bcs_file_2k VARY mxmyz
!-----
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Inf Isy Str Furth ATZ Hvk Npr More
7 0 0 0 0 0 0 10 10 0 2 0 0 0.000 0 7 0
!
P_C4/ncc number:130.433 <--Magnetic Space group symbol (BNS/UNI symbol & number)
Transform to standard: 1/2a+1/2b,-1/2a+1/2b,c;0,1/4,0
Parent Space Group: I4/mcm IT_number: 140
Transform from Parent: 2a,2b,c;0,0,0
! Nsym Cen N_Clat N_Ant
16 0 1 2
!
! Centring vectors
0.50000 0.50000 0.00000
! Anti-Centring vectors
0.00000 0.50000 0.00000
0.50000 0.00000 0.00000
! Symmetry operators
1 x,y,z,+1
2 -x,-y,-z,-1
3 y,-x,-z,-1
4 x,y,-z,-1
5 -y,x,z,+1
6 y,-x,z,+1
7 -y,x,-z,-1
8 -x,-y,z,+1
9 -y,-x,z+1/2,+1
10 y,x,z+1/2,+1
11 y,x,-z+1/2,-1
12 -y,-x,-z+1/2,-1
13 -x,y,-z+1/2,-1
14 x,-y,-z+1/2,-1
15 -x,y,z+1/2,+1
16 x,-y,z+1/2,+1
!
!Atom Type Mag Vek X Y Z Biso Occ N_type Spc /Line below:Codes
! Rx Ry Rz beta22 beta33 beta12 beta13 beta23 / Line below:Codes
Ba1_1 Ba 1 0 0.00000 0.00000 0.25000 0.00000 0.12500 0 0 #
0.00 0.00 0.00 0.00 0.00 0.00 0.00
Ba1_2 Ba 1 0 0.25000 0.25000 0.75000 0.00000 0.12500 0 0 #
0.00 0.00 0.00 0.00 0.00 0.00 0.00
Nd1 JND3 1 0 0.08700 0.33700 0.00000 0.00000 0.50000 1 0 #
0.00 0.00 0.00 0.00 0.00 0.00 0.00
2.00000 2.00000 0.00000 0.00000 0.00000 0.00000 0.00000 <-MagPar
0.00 0.00 0.00 0.00 0.00 0.00 0.00
Zn1 Zn 1 0 0.00000 0.25000 0.25000 0.00000 0.25000 0 0 #
0.00 0.00 0.00 0.00 0.00 0.00 0.00
  
```

Perform the refinement on the BNZO_0p25.dat data

Constrain $m_x = -m_y$ to force the moments orthogonal to Nd bonds

!										
!Atom	Typ	Mag	Vek	X	Y	Z	Biso	Occ	N_type	Spc/Fftype /Line be
! Rx	Ry	Rz	Ix	Iy	Iz	MagPh	/ Line below:Codes			
! beta11	beta22	beta33	beta12	beta13	beta23	/ Line below:Codes				
Ba1_1	Ba	1	0	0.00000	0.00000	0.25000	0.00000	0.12500	0	0 #
				0.00	0.00	0.00	0.00	0.00		
Ba1_2	Ba	1	0	0.25000	0.25000	0.75000	0.00000	0.12500	0	0 #
				0.00	0.00	0.00	0.00	0.00		
Nd1	JND3	1	0	0.08700	0.33700	0.00000	0.00000	0.50000	1	0 #
				0.00	0.00	0.00	0.00	0.00		
	-1.23859	1.23859	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	<-MagPar	
	-21.00	21.00	0.00	0.00	0.00	0.00	0.00	0.00		
Zn1	Zn	1	0	0.00000	0.25000	0.25000	0.00000	0.25000	0	0 #
				0.00	0.00	0.00	0.00	0.00		
O1_1	O	1	0	0.00000	0.00000	0.00000	0.00000	0.12500	0	0 #
				0.00	0.00	0.00	0.00	0.00		
O1_2	O	1	0	0.25000	0.25000	0.50000	0.00000	0.12500	0	0 #
				0.00	0.00	0.00	0.00	0.00		
O2	O	1	0	0.17729	0.42729	0.13111	0.00000	1.00000	0	0 #
				0.00	0.00	0.00	0.00	0.00		



The double k-model consists of uniform moment on Nd sites with ferromagnetic dimers.

Creating the 2k- order moder using Irreps with SARAh

Calculate the Irreps and Basis vectors for each k vector contribution to the double-k : $(\frac{1}{2}, \frac{1}{2}, 0)$ & $(\frac{1}{2}, -\frac{1}{2}, 0)$

Edit the PCR file to combine the BV for both k vectors. See the provided PCR
“Irreps_2k_BNZO.pcr”

SARAh webRefine – FullProf

Three pieces of advice for using SARAh webRefine : 1. change your browser settings to allow you to select where you save downloads (and overwrite files). 2. when you click <evaluate>, it will look like nothing is happening for a few seconds. Look in the tab '4. Help and Strategies' for more information. 3. if editing a pcr file creates an error, try moving your file so that its path contains no special characters; special characters and those with PHP commands, etc can fail validation checks.

-Andrew (February 2022)



1. Conventional basis vectors (as projected)	2. Stationary vector combinations	3. Exchange multiplets	4. Help and strategies
--	-----------------------------------	------------------------	------------------------

Method 2. Basis vectors combined according to stationary vectors

Select command (generate template for magnetic phase for pcr, edit pcr with magnetic phase present):

1. powder format 2. make template pcr

☐ Nd3 Γ_1 η_1 ψ_1	☐ Nd3 Γ_4 η_1 ψ_2	☐ Nd3 Γ_8 η_1 ψ_1	☐ Nd3_2 Γ_2 η_1 ψ_2	☐ Nd3_2 Γ_5 η_1 ψ_1
☐ Nd3 Γ_2 η_1 ψ_1	☐ Nd3 Γ_5 η_1 ψ_1	☐ Nd3 Γ_8 η_1 ψ_2	☐ Nd3_2 Γ_3 η_1 ψ_1	☐ Nd3_2 Γ_6 η_1 ψ_1
☐ Nd3 Γ_3 η_1 ψ_1	☐ Nd3 Γ_6 η_1 ψ_1	☐ Nd3_2 Γ_1 η_1 ψ_1	☐ Nd3_2 Γ_3 η_1 ψ_2	☐ Nd3_2 Γ_7 η_1 ψ_1
☐ Nd3 Γ_3 η_1 ψ_2	☐ Nd3 Γ_7 η_1 ψ_1	☐ Nd3_2 Γ_1 η_1 ψ_2	☐ Nd3_2 Γ_4 η_1 ψ_1	☐ Nd3_2 Γ_8 η_1 ψ_1
☐ Nd3 Γ_4 η_1 ψ_1	☐ Nd3 Γ_7 η_1 ψ_2	☐ Nd3_2 Γ_2 η_1 ψ_1	☐ Nd3_2 Γ_4 η_1 ψ_2	

(Your browser should be set to ask for the download location so the pcr file can be overwritten. Please look in '4. Help and strategies' for an explanation/help.)

Submit

Table. Stationary vector groups (stationary vectors, symmetry groups, and symmetry operations):

Stationary vector Γ_i	Black and white point group $m_i = (a)$	Normal point group D 2 . 222	Normal symmetry operations 1 2 3 4	Primed symmetry operations (i)
---------------------------------	--	---------------------------------	---------------------------------------	-----------------------------------

```
I -1 <--Space group symbol for hkl generation
! Nsym Cen Laue Ireps N_Bas
2 1 1 -2 1
! Real(0)-Imaginary(1) indicator for Ci
0
!
SYMM X, Y, Z
BASR 1 -1 0
BASI 0 0 0
BASR 1 1 0
BASI 0 0 0
SYMM -X+1, -Y+1, Z
BASR -1 1 0
BASI 0 0 0
BASR -1 -1 0
BASI 0 0 0
!
!Atom Typ Mag Vek X Y Z Biso Occ C1 C2 C3
! C4 C5 C6 C7 C8 C9 MagPh
ND1 JND3 1 1 0.17363 0.67363 0.00000 0.10000 1.00000 1.135 0.000 0.000 #
0.000 0.000 0.00 0.00 0.00 0.00 0.00 0.00 11.00 0.00 0.00
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
ND2 JND3 2 2 0.32637 0.17363 0.00000 0.10000 1.00000 1.135 0.000 0.000 #
0.000 0.000 0.00 0.00 0.00 0.00 0.00 0.00 11.00 0.00 0.00
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
!-----> Profile Parameters for Pattern # 1 ----> Phase # 2
! Scale Shape1 Bov Str1 Str2 Str3 Strain-Model
0.3069980 0.00000 0.00000 0.00000 0.00000 0.00000 0
21.00000 0.000 0.000 0.000 0.000 0.000
! U V W X Y GauSiz Lors
-0.075852 0.000000 0.046673 0.000000 0.000000 0.000000 0.00
0.00 0.00 0.00 0.00 0.00 0.00
! a b c alpha beta gamma # Cell Info
6.736217 6.736217 11.519499 90.000000 90.000000 90.000000
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
! Pref1 Pref2 Asy1 Asy2 Asy3 Asy4 S_L D_L
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
! Propagation vectors:
0.5000000 0.5000000 0.0000000 Propagation Vector 1
0.0000000 0.0000000 0.0000000
0.5000000 -0.5000000 0.0000000 Propagation Vector 2
0.0000000 0.0000000 0.0000000
! 2Th1/TOF1 2Th2/TOF2 Pattern to plot
```

Creating the 2k- order model using ISODISTORT (basis functions refinement under magnetic space group constraints)

<https://iso.byu.edu/isodistortform.php>

1.)

Types of distortions to be considered [Change](#) [?](#)

strain: ☐

Displacive: all ☐ none ☐ Ba2+ ☐ Nd3+ ☐ Zn2+ ☐ O2- ☒

Occupational: all ☐ none ☐ Ba2+ ☐ Nd3+ ☐ Zn2+ ☐ O2- ☐

Magnetic: all ☐ none ☐ Ba2+ ☐ Nd3+ ☒ Zn2+ ☐ O2- ☐

Rotational: all ☐ none ☐ Ba2+ ☐ Nd3+ ☐ Zn2+ ☐ O2- ☐

Important: You must click on Change to implement any changes in the above type of distortion

2.)

Method 2: General method - search over specific k points [OK](#) [?](#)

Specify k point: a= b= g= # of

Change number of superposed IRs: [Change](#) [?](#)

3.)

Choose an IR and OPD (optional):

IR:

4.)

Finish selecting the distortion mode by choosing an order parameter direction [?](#)

- ☒ P1 (a;a) 130.433 P4/ncc.1'_C[rP4/mcc], basis={{(1,-1,0),(1,1,0),(0,0,1)}, origin=(-1,1/2,0), s=4, i=4, k-active= (1/2,1/2,0),(1/2,1/2,1)}
- ☐ P3 (a;0) 64.480 Cmca.1'_A[Fmmm], basis={{(1,-1,0),(0,0,-1),(1,1,0)}, origin=(1/2,0,0), s=2, i=4, k-active= (1/2,1/2,0)}
- ☐ C1 (a;b) 56.375 Pccn.1'_C[Cccm], basis={{(-1,1,0),(-1,-1,0),(0,0,1)}, origin=(-1/2,0,0), s=4, i=8, k-active= (1/2,1/2,0),(1/2,1/2,1)}

← single k model

← double-k model

[OK](#)

5.)

IR: mX2-, mk13t8

P1 (a;a) 130.433 P4/ncc.1'_C[rP4/mcc], basis={{(1,-1,0),(1,1,0),(0,0,1)}, origin=(-1,1/2,0), s=4, i=4, k-active= (1/2,1/2,0),(1/2,1/2,1)}

Lattice parameters of undistorted supercell: a=9.52645, b=9.52645, c=11.51950, alpha=90.00000, beta=90.00000, gamma=90.00000

[interactive viewer](#)

☐ Save interactive distortion [?](#) ☐ Save interactive diffraction [?](#) ☐ CIF file [?](#) ☐ Distortion file [?](#) ☐ Domains [?](#) ☐ Primary order parameters [?](#)

☐ Complete modes details [?](#) ☐ TOPAS.STR [?](#) ☒ FULLPROF.pcr [?](#) ☐ IR matrices ☐ Subgroup tree [OK](#)

Enter mode and strain amplitudes: [?](#)

Creating the 2k- order moder using ISODISTORT (cont)

- Edit the saved PCR file to update the input lines and the profile parameters
- the provided PCR file prepared using this method is: **"Isodistort_2k_BNZO.pcr"**

```
.
AMPLIMODES for FullProf      FIX xyz
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth      ATZ      Nvk Npr More
  7  0  0 0.0 0.0 1.0 -6  0  2  0  5      9139.152  0  7  0
!
P4/ncc.1'_C[rP4/mcc] number: 130.433  <--Magnetic Space Group Symbol (UNI symbol and BNS number)
Transform to standard: 1/2a-1/2b,1/2a+1/2b,c;0,0,0  <--Basis transformation from alt setting to standard BNS
Parent space group: I4/mcm IT_number: 140  <--Nonmagnetic Parent Group
Transform from Parent: 2a,2b,c;1,1/2,0  <--Basis transformation from parent to current setting
!
!Atom  Typ  Mag Vek  X      Y      Z      Bis0  Occ  N_type  Spc/Fftype /Line below:Codes
!      Rx      Ry      Rz      Ix      Iy      Iz      MagPh / Line below:Codes
!      beta11  beta22  beta33  beta12  beta13  beta23 / Line below:Codes
Ba1_1  BA      0  0      0.50000  0.75000  0.25000  0.50000  0.25000  0  1
          0.00      0.00      0.00      0.00      0.00      0.00      0.00
Ba1_2  BA      0  0      0.25000  0.00000  0.75000  0.50000  0.25000  0  1
          0.00      0.00      0.00      0.00      0.00      0.00      0.00
Nd1_1  JND3      1  0      0.58699  0.08699  0.00000  0.50000  1.00000  1  2
          0.00      0.00      0.00      0.00      0.00      0.00      0.00
          0.00000  0.00000  0.00000  0.00000  0.00000  0.00000  0.00000 <-MagPar
          0.00      0.00      0.00      0.00      0.00      0.00      0.00
```

```
! Basis Vectors of Magnetic Symmetry Modes for each atom
M_MODES 2
! Nm Atm Irrep      Mx      My      Mz      Coeff
  1 Nd1_1 mX2-      0.013100 -0.013100  0.000000  1.000000
  2 Nd1_1 mX2-      0.013100  0.013100  0.000000  1.000000
```

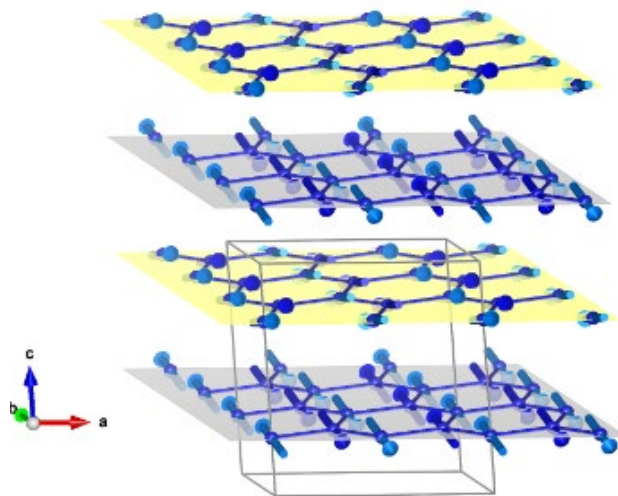
```
! Amplitudes of Magnetic Symmetry Modes
MA_MODES 2
      A4_mX2-      3.907968      21.000000
      A5_mX2-      3.907968      21.000000
```

- Get the refined moment value from *.sum or *.out file:

=> Magnetic Moment Components and Standard Deviations

Atom	Mx	sMx	My	sMy	Mz	sMz	M	sM
Nd1_1	1.3794	0.0147	0.0000	0.0147	0.0000	0.0000	1.3794	0.0015

3-k magnetic structure in honeycomb system $\text{Na}_2\text{Co}_2\text{TeO}_6$



$\text{Na}_2\text{Co}_2\text{TeO}_6$ (#1.645)

[view in Jmol](#)

[Download mcif file](#)

[Download vesta file \(all atoms\)](#)

[Download vesta file \(magnetic atoms only\)](#)

[submit to STRCONVERT](#)

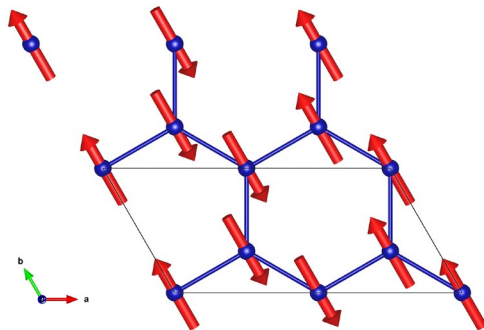
Orders with $k = (1/2, 0, 0)$ below ~ 25

Single k structure consist of a zigzag-type order described by the MSG

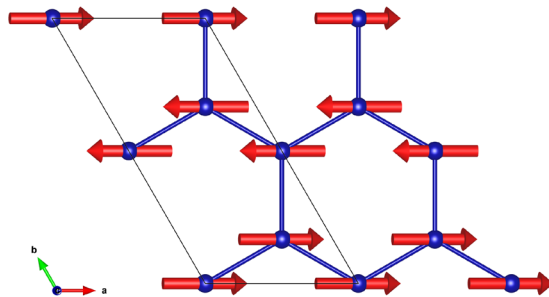
$P_C2_12_12_1$ (# 19.29) in $(2a,b,c)$ lattice

Phys. Rev. B **104**, 184415 (2021)

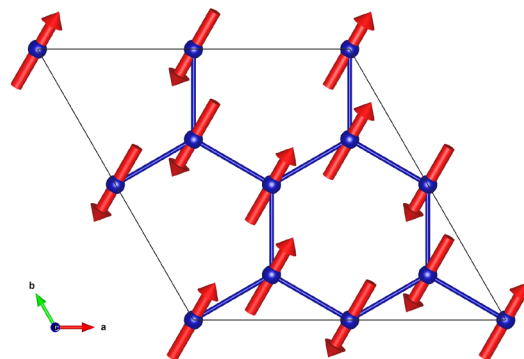
$k_1 = (1/2, 0, 0),$



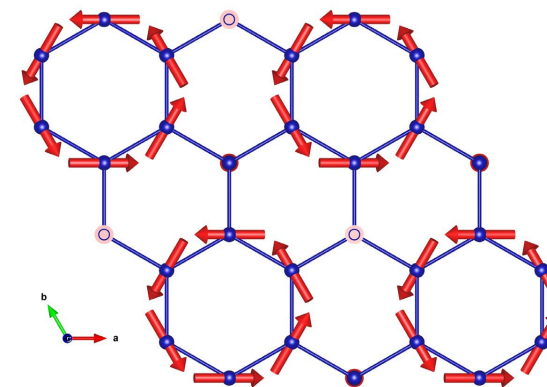
$k_2 = (0, 1/2, 0),$



$k_3 = (-1/2, 1/2, 0),$



Supposition of $k_1 + k_2 + k_3$

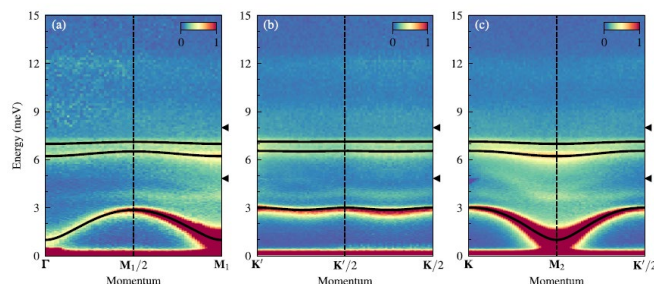
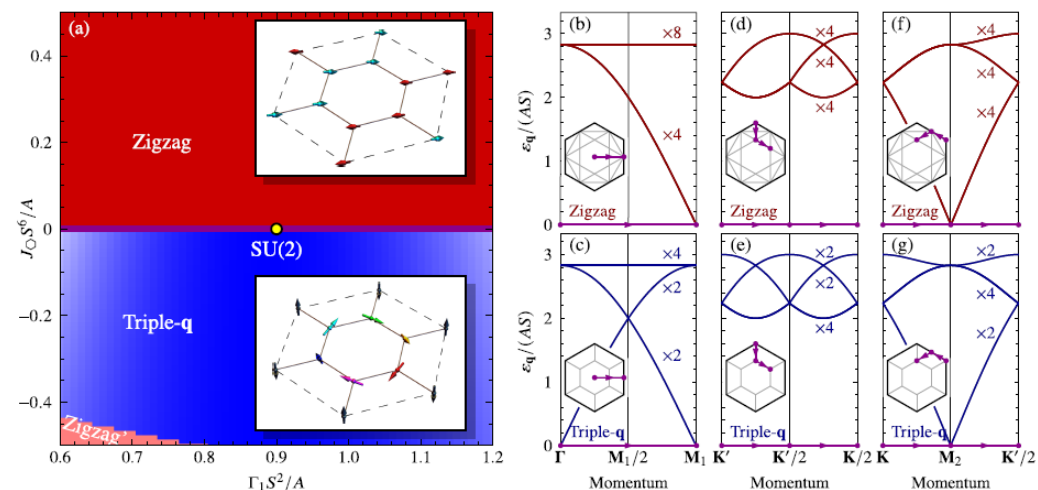


Experimental evidences of the triple-k order in $\text{Na}_2\text{Co}_2\text{TeO}_6$

Krüger et al. Phys. Rev. Lett. 131, 146702 (2023)

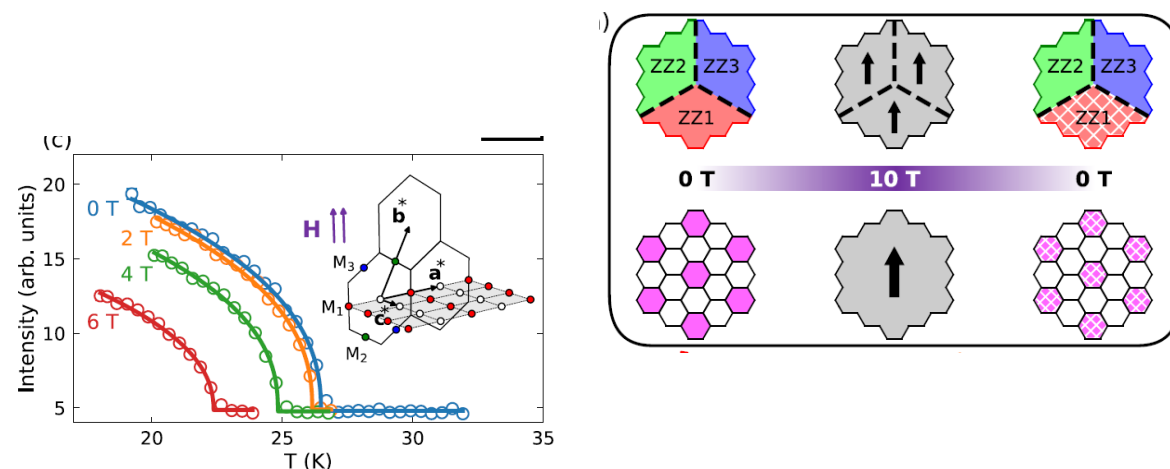
the magnetic Brillouin zone in a multi-q state differs from those of the corresponding single-q states.

→ different symmetries of the magnetic excitations

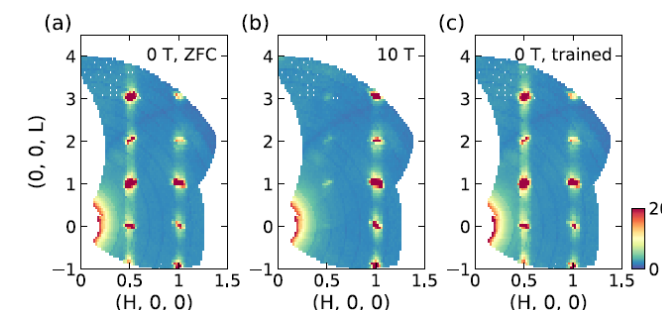


Yao et al. Phys. Rev. Res. **5**, L022045 (2023)

External perturbation (e.g., in-plane magnetic field, strain, etc.) can be expected to selectively populate the domains if the zigzag ground state is realized



field is unable to repopulate the supposed zigzag domains



Explore the possible magnetic models compatible a triple -k : (1/2, 0, 0) , (1/2, 0, 0) and (-1/2, 1/2, 0) using the **k-SUBGROUPSMAG**

k-Subgroupsmag: Magnetic subgroups compatible with some given propagation vector(s) or a supercell.

k-Subgroupsmag

The program *k-Subgroupsmag* provides the possible magnetic subgroups of the space group of a paramagnetic phase (gray group) which are possible for a magnetic ordering having a known propagation vector. The program provides the set of magnetic subgroups or a graph showing the subgroup-tree (grouped into conjugacy classes). In both cases, more information about the classes or subgroups can be obtained.

Other alternatives for the input of the program:

- An alternative parent (non gray) magnetic group can be chosen.
- Instead of the whole set of subgroups, the output can be limited to subgroups having a chosen common subgroup of lowest symmetry, common point group of lowest symmetry, or groups which belong to a specific crystal class.
- Further restrictions on the subgroup list/graph considering physical

Enter the serial number of the space group of the parent paramagnetic phase:

choose it 182

Choose an alternative magnetic group

Introduce the magnetic wave vector(s)

(Give the components of the wave vectors in a fractional form, n/m)

k_{1x} 0.5 k_{1y} 0 k_{1z} 0
k_{2x} 0 k_{2y} -0.5 k_{2z} 0
k_{3x} -0.5 k_{3y} 0.5 k_{3z} 0

Show the independent vectors of the star

☐ Choose the whole star of the propagation vector

(Give the r

k_{1x} 0.5 k_{1y} 0 k_{1z} 0
k_{2x} k_{2y} k_{2z}
k_{3x} k_{3y} k_{3z}

Show the independent vectors of the star

☒ Choose the whole star of the propagation vector

P₆3221' (N. 182)

P1 (N. 1.1)

(0.5,0,0),(0,-0.5,0),(-0.5,0.5,0)

List of subgroups that fulfill the given conditions

Get the subgroup-graph

N	Group Symbol	Transformation matrix	Group-Subgroup index	Other members of the Conjugacy Class	irreps	Magnetic structure models (MAGMODELIZE)
1	P ₆ 3'2'2' (No. 182.183)	$\begin{pmatrix} 2 & 0 & 0 & 1 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=4x2	Conjugacy Class	Get irreps	☒
2	P ₆ 3'22' (No. 182.182)	$\begin{pmatrix} 2 & 0 & 0 & 1 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=4x2	Conjugacy Class	Get irreps	☐
3	P ₆ 3'2'2 (No. 182.181)	$\begin{pmatrix} 2 & 0 & 0 & 1 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=4x2	Conjugacy Class	Get irreps	☐
4	P ₆ 322 (No. 182.179)	$\begin{pmatrix} 2 & 0 & 0 & 1 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	8=4x2	Conjugacy Class	Get irreps	☐
5	P ₆ 3' (No. 173.131)	$\begin{pmatrix} 2 & 0 & 0 & 1 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	16=4x4	Conjugacy Class	Get irreps	☐
6	P ₆ 3 (No. 173.129)	$\begin{pmatrix} 2 & 0 & 0 & 1 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	16=4x4	Conjugacy Class	Get irreps	☐

Load crystallographic information from “nuc_Na2Co2TeO6.cif”

Parent space group: P₆322 (No. 182)

Lattice parameters (Angstroms and degrees): a=5.25870, b=5.25880, c=11.16980, alpha=90.000, beta=90.000, gamma=120.0

Atoms: Please select the magnetic ones

N	Atom name	Atom type	Wyckoff Position	Coordinates	Occupancies	Magnetic?
1	Te1	Te	2c	0.33333 0.66667 0.25000	1	☐
2	Co1	Co	2b	0.00000 0.00000 0.25000	1	☒
3	Co2	Co	2d	0.66667 0.33333 0.25000	1	☒
4	O1	O	12i	0.64910 -0.02250 0.34540	1	☐
5	Na1	Na	12i	0.43000 0.59400 -0.07700	0.093	☐
6	Na2	Na	12i	0.69900 0.06650 -0.00210	0.258	☐
7	Na3	Na	2a	0.00000 0.00000 0.00000	0.38	☐

Select the MSG $P6_32'2'$ (#182.183). Note that the magnetic lattice becomes $(2a, 2a, c)$

Maximal subgroups which allow non-zero magnetic moments for at least one atom are coloured

N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	$P6_32'2' \text{ (#182.183)}$ Go to a subgroup	$\begin{pmatrix} 2 & 0 & 0 & 1 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	<i>Systematic absences</i> MAGNEXT <i>Tensor properties</i> MTENSOR	Show

Create a PCR from MCIF using the FullProf ToolBar

Atomic positions, Wyckoff positions and Magnetic Moments

N	Atom	Occupancy	New WP	Multiplicity	Magnetic moment	Values of M_x, M_y, M_z
1	Te1_1 Te 0.16667 0.33333 0.25000	1.	$(1/6, 1/3, 1/4 \mid 0, 0, m_z)$ $(5/6, 2/3, 3/4 \mid 0, 0, m_z)$	2	-	-
	Te1_2 Te 0.33333 0.16667 0.75000	1.	$(1/3, 1/6, 3/4 \mid m_x, m_y, m_z)$ $(1/6, 5/6, 1/4 \mid 0, m_x, m_z)$ $(1/3, 2/3, 3/4 \mid -m_x, 0, m_z)$ $(2/3, 1/3, 1/4 \mid m_x, 0, m_z)$ $(5/6, 1/6, 3/4 \mid 0, -m_x, m_z)$ $(2/3, 5/6, 1/4 \mid -m_x, -m_y, m_z)$	6	-	-
2	Co1_1 Co 0.00000 0.00000 0.25000	1.	$(0, 0, 1/4 \mid m_x, 0, m_z)$ $(0, 0, 3/4 \mid -m_x, 0, m_z)$ $(0, 1/2, 1/4 \mid -m_x, -m_y, m_z)$ $(0, 1/2, 3/4 \mid m_x, m_y, m_z)$ $(1/2, 1/2, 1/4 \mid 0, m_x, m_z)$ $(1/2, 1/2, 3/4 \mid 0, -m_x, m_z)$	6	$(M_x, 0, M_z)$	$M_x = \begin{matrix} \boxed{1} \\ \boxed{0.5} \end{matrix}$ $M_z = \begin{matrix} \boxed{1} \\ \boxed{0.5} \end{matrix}$
	Co1_2 Co 0.50000 0.00000 0.25000	1.	$(1/2, 0, 1/4 \mid 0, 0, m_z)$ $(1/2, 0, 3/4 \mid 0, 0, m_z)$	2	$(0, 0, M_z)$	$M_z = \begin{matrix} \boxed{1} \\ \boxed{0.5} \end{matrix}$
3	Co2_1 Co 0.16667 0.33333 0.75000	1.	$(1/6, 1/3, 3/4 \mid 0, 0, m_z)$ $(5/6, 2/3, 1/4 \mid 0, 0, m_z)$	2	$(0, 0, M_z)$	$M_z = \begin{matrix} \boxed{1} \\ \boxed{0.5} \end{matrix}$
	Co2_2 Co 0.33333 0.16667 0.25000	1.	$(1/3, 1/6, 1/4 \mid m_x, m_y, m_z)$ $(1/6, 5/6, 3/4 \mid 0, m_x, m_z)$ $(1/3, 2/3, 1/4 \mid -m_x, 0, m_z)$ $(2/3, 1/3, 3/4 \mid m_x, 0, m_z)$ $(5/6, 1/6, 1/4 \mid 0, -m_x, m_z)$ $(2/3, 5/6, 3/4 \mid -m_x, -m_y, m_z)$	6	(M_x, M_x, M_z)	$M_x = \begin{matrix} \boxed{1} \\ \boxed{0.5} \end{matrix}$ $M_z = \begin{matrix} \boxed{1} \\ \boxed{0.5} \end{matrix}$
4	O1_1 O 0.32455 0.48875 0.34540	1.	$(x, y, z \mid m_x, m_y, m_z)$ $(-x, -y, z+1/2 \mid -m_x, -m_y, m_z)$ $(x-y, -y, -z \mid -m_x+m_y, m_y, m_z)$ $(-x+y, -z+1/2 \mid m_x-m_y, -m_y, m_z)$ $(-x-y, -x+1/2, z \mid -m_x+m_y, -m_x, m_z)$ $(x-y, -x+1/2, z+1/2 \mid m_x-m_y, m_x, m_z)$ $(-x, -x+y+1/2, -z \mid m_x, m_x-m_y, m_z)$ $(x, -x+y+1/2, -z+1/2 \mid -m_x, -m_y+m_y, m_z)$ $(-y+1/2, x-y+1/2, z \mid -m_y, m_x-m_y, m_z)$ $(y+1/2, -x+y+1/2, z+1/2 \mid m_y, -m_x+m_y, m_z)$ $(y+1/2, x+1/2, -z \mid -m_y, -m_x, m_z)$ $(-y+1/2, -x+1/2, -z+1/2 \mid m_y, m_x, m_z)$	12	-	-

```

COMM PCR-model generated by mCIF_to_PCR for: bcs_3K-model
! Current global Chi2 (Bragg contrib.) = 9999999.0
! Files => DAT-file: , PCR-file:
! Job Npr Nph Nba Nex Nsc Nor Dum Iwg Ilo Ias Res Ste Nre Cry Uni Cor Opt Aut
1 7 1 6 2 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
!
! Ipr Ppl Ioc Mat Pcr Ls1 Ls2 Ls3 NLI Prf Ins Rpa Sym Hkl Fou Sho Ana
3 0 1 0 1 0 0 0 0 0 -3 10 0 0 0 0 0 0 0
!
! Lambda1 Lambda2 Ratio Bkpos Wdt Cthm muR AsyLim Rpolarz 2nd-muR -> Patt# 1
1.000000 1.900000 0.00000 30.000 15.0000 0.00000 0.0000 180.00 0.0000 0.0000
!
! INCY Eps R_at R_an R_pr R_gl Thmin Step Thmax PSD Sent0
1 0.02 1.00 1.00 1.00 1.00 2.0000 0.0200 130.0000 0.000 0.000
!
! 2Theta/TOF/E(Kev) Background for Pattern# 1
2.00 100.00 0.00
20.00 100.00 0.00
40.00 100.00 0.00
80.00 100.00 0.00
100.00 100.00 0.00
130.00 100.00 0.00
!
! Excluded regions (LowT HighT) for Pattern# 1
0.00 2.00
130.00 180.00
!
! 0 !Number of refined parameters
!
! Zero Code SyCos Code SySin Code Lambda Code MORE ->Patt# 1
0.00 0.00 0.00 0.00 0.00 0.00 0.00000 0.00 0
!-----
! Data for PHASE number: 1 ==> Current R_Bragg for Pattern# 1: 999.00
!-----
Nuclear and Magnetic Structure of: bcs_3K-model VARY mxmymz
!
! Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth ATZ Nvk Npr More
20 0 0 0.0 0.0 1.0 10 0 2 0 0 0.000 0 7 0
!
P6_32'2' number:182.183 <--Magnetic Space group symbol (BNS/UNI symbol & number)
Transform to standard: a,b,c;1/2,0,0
Parent Space Group: P6_32 IT_number: 182
Transform from Parent: 2a,2b,c;0,0,0
! Nsym Cen N_Clat N_Ant
12 0 0 0
!
! Symmetry operators
1 x,y,z,+1
2 x-y,-y,-z,-1
3 -x+y,-x+1/2,z,+1
4 -x,-x+y+1/2,-z,-1
5 -x+y,y,-z+1/2,-1

```

There is no need to adapt instrumental configuration in the PCR file because the data was created from the same default setting. Change the **Job** to "1" (for Rietveld fitting) and "**NCY**" to 10. Also remove **VARY mxmymz** comment.

Perform a constrained refinement on the “data_na2co2teo6_1k_model.dat” data

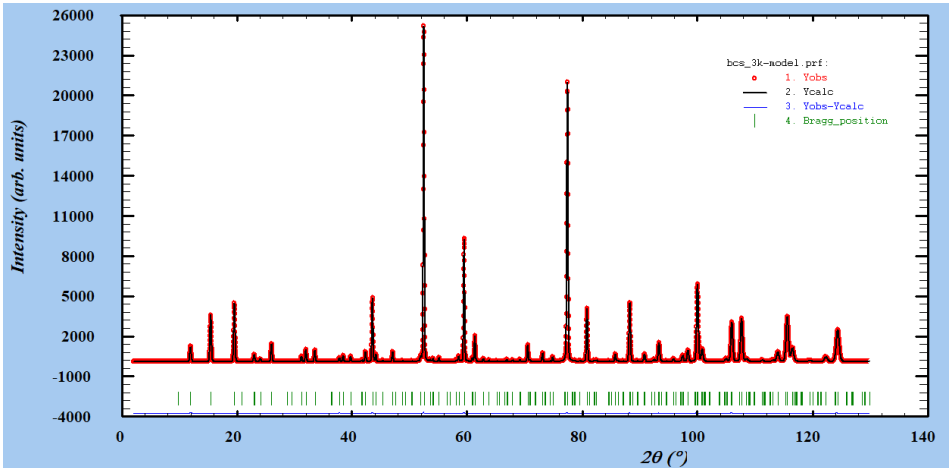
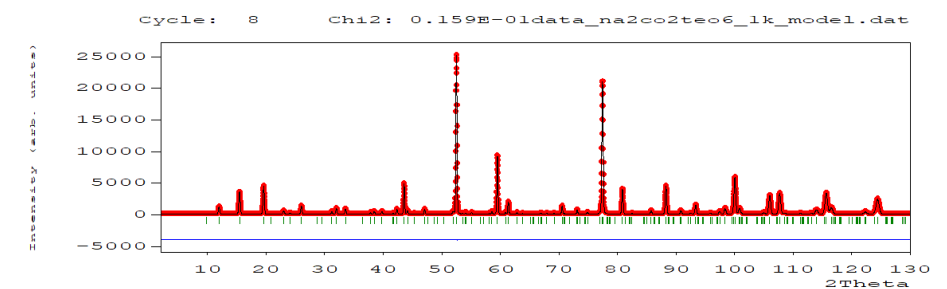
- Constrain the in-plane and out of plane moment components to be equal for all sites.
- Refine the scale factor since the size of unit cell is different.

11 y+1/2, -x+y+1/2, z+1/2, +1
12 -y+1/2, -x+1/2, -z+1/2, -1
!

!Atom	Typ	Mag Vek	X	Y	Z	Biso	Occ	N_type	Spc/Fftype	/Line below:Codes
! Rx	Ry	Rz	Ix	Iy	Iz	MagPh	/ Line below:Codes			
Te1_1	Te	1 0	0.16667	0.33333	0.25000	0.00000	0.16667	0	0	#
			0.00	0.00	0.00	0.00	0.00			
Te1_2	Te	1 0	0.33333	0.16667	0.75000	0.00000	0.50000	0	0	#
			0.00	0.00	0.00	0.00	0.00			
Co1_1	MC02	1 0	0.00000	0.00000	0.25000	0.00000	0.50000	1	0	#
			0.00	0.00	0.00	0.00	0.00			
	2.30936	0.00000	0.47022	0.00000	0.00000	0.00000	0.00000	<-MagPar		
	11.00	0.00	31.00	0.00	0.00	0.00	0.00			
Co1_2	MC02	1 0	0.50000	0.00000	0.25000	0.00000	0.16667	1	0	#
			0.00	0.00	0.00	0.00	0.00			
	0.00000	0.00000	-0.47022	0.00000	0.00000	0.00000	0.00000	<-MagPar		
	0.00	0.00	-31.00	0.00	0.00	0.00	0.00			
Co2_1	MC02	1 0	0.16667	0.33333	0.75000	0.00000	0.16667	1	0	#
			0.00	0.00	0.00	0.00	0.00			
	0.00000	0.00000	0.47022	0.00000	0.00000	0.00000	0.00000	<-MagPar		
	0.00	0.00	31.00	0.00	0.00	0.00	0.00			
Co2_2	MC02	1 0	0.33333	0.16667	0.25000	0.00000	0.50000	1	0	#
			0.00	0.00	0.00	0.00	0.00			
	2.30936	2.30936	-0.47022	0.00000	0.00000	0.00000	0.00000	<-MagPar		
	11.00	11.00	-31.00	0.00	0.00	0.00	0.00			
01_1	0	1 0	0.32455	0.48875	0.34540	0.00000	1.00000	0	0	#
			0.00	0.00	0.00	0.00	0.00			
01_2	0	1 0	0.51125	0.83580	0.34540	0.00000	1.00000	0	0	#
			0.00	0.00	0.00	0.00	0.00			
01_3	0	1 0	0.16420	0.67545	0.34540	0.00000	1.00000	0	0	#
			0.00	0.00	0.00	0.00	0.00			
01_4	0	1 0	0.82455	0.48875	0.34540	0.00000	1.00000	0	0	#

```
FullProf Program
=> Expected : 5.08 1.9234
=> Conventional Rietveld R-factors for Pattern: 1
=> Rp: 0.363 Rwp: 0.784 Rexp: 6.21 Chi2: 0.159E-01
=> Global user-weighted Chi2 (Bragg contrib.): 0.1635E-01
=> ----- Pattern# 1
=> Phase: 1
=> Bragg R-factor: 0.1985
=> RF-factor : 0.1664
=> Nuclear R-factor: 0.1985
=> Magnetic R-factor: 0.9549
=> Pure Magnetic R-factor: 0.1998E-20
=> Normal end, final calculations and writing...
=> Contribution to Yi for phase: 1

=> CPU Time: 5.244 seconds
=> 0.087 minutes
=> END Date:19/07/2024 Time => 21:37:49.705
```



Triple-k order in $\text{Na}_2\text{Co}_2\text{TeO}_6$

each of the two non-identical Co sites of the parent structure is divided into two additional magnetic sites (with multiplicities 6 and 2), leading to 4 magnetic sublattices.

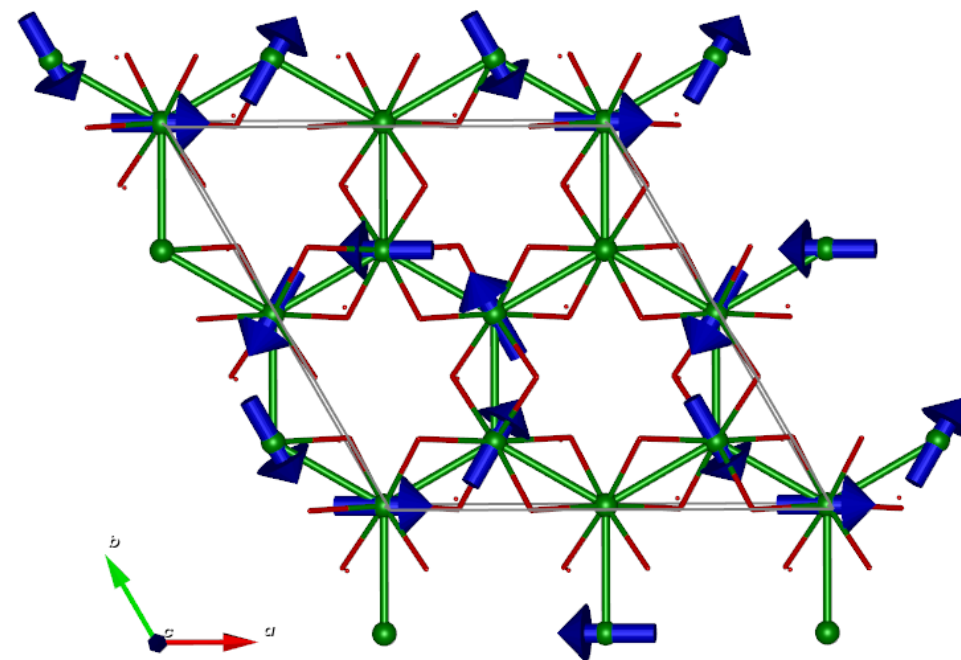
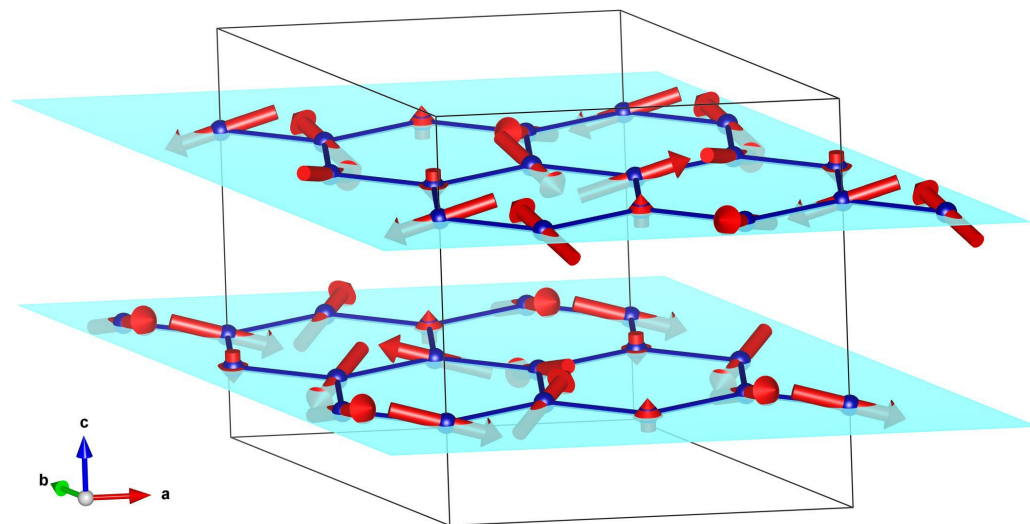
$$m_{\text{Co11}} = (2.32, 0, -0.5) \mu_B,$$

$$m_{\text{Co12}} = (0, 0, 0.5) \mu_B,$$

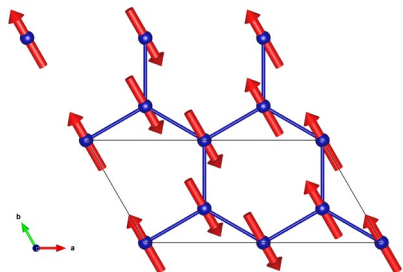
$$m_{\text{Co21}} = (2.32, 2.32, 0.5) \mu_B$$

$$m_{\text{Co22}} = (0, 0, -0.5) \mu_B.$$

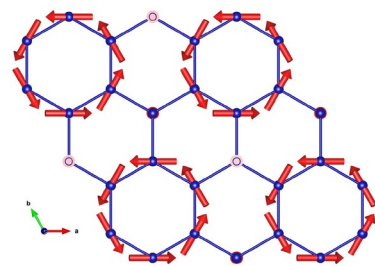
Use FullProf Studio or Vesta to visualize



Constructing the 3k-structure of $\text{Na}_2\text{Co}_2\text{TeO}_6$, using ISODISTORT



Single $k = (1/2, 0, 0)$,
zigzag-type order
described by
 $P_{C2_12_12_1}$ (# 19.29)



Triple - k
described by
 $P6_32'2'$ (#182.183)

- Load crystallographic information from “[nuc_Na2Co2TeO6.cif](#)”
- Select magnetic distortion for Co
- Use Method 2 and select M ($1/2, 0, 0$)

ISODISTORT: search

Space Group: 182 P6₃22 D6-6, Lattice parameters: a= 5.25880, b= 5.25880, c= 11.16980, alpha= 90.00000, beta= 90.00000, gamma= 120.00000
Default space-group preferences: monoclinic axes a(b)c, monoclinic cell choice 1, orthorhombic axes abc, origin choice 2, hexagonal axes, SSG standard setting
Te1 2c (1/3,2/3,1/4), Co1 2b (0,0,1/4), Co2 2d (1/3,2/3,3/4), O1 12i (x,y,z), x=-0.35090, y=-0.02250, z= 0.34540, Na1 12i (x,y,z), x= 0.43000, y=-0.40600, z=-0.07700,
Include displacive O, magnetic Co distortions

Types of distortions to be considered [Change](#) [?](#)

strain: ☐
Displacive: all ☐ none ☐ Te ☐ Co ☐ O ☒ Na ☐
Occupational: all ☐ none ☐ Te ☐ Co ☐ O ☐ Na ☐
Magnetic: all ☐ none ☐ Te ☐ Co ☒ O ☐ Na ☐
Rotational: all ☐ none ☐ Te ☐ Co ☐ O ☐ Na ☐

Important: You must click on Change to implement any changes in the above type of distortions to be considered.

Method 1: Search over all special k points [OK](#) [?](#)

Crystal system(s): triclinic ☐ monoclinic ☐ orthorhombic ☐ tetragonal ☐ trigonal ☐ hexagonal ☐ cubic ☐

Space-group symmetry: no choice ☐ Conventional lattice: no choice ☐ Primitive lattice: no choice ☐

Method 2: General method - search over specific k points [OK](#) [?](#)

Specify k point: M, k12 (1/2,0,0) ☐ a= b= g= # of independent incommensurate modulations=

Change number of superposed IRs: 1 [Change](#) [?](#)

Important: You must click on Change to implement any changes in the number of superposed IRs.

ISODISTORT: irreducible representation

Space Group: 182 P6₃2 D6-6, Lattice parameters: a= 5.25880, b= 5.25880, c= 11.16980, alpha= 90.00000, beta= 90.00000
Default space-group preferences: monoclinic axes a(b)c, monoclinic cell choice 1, orthorhombic axes abc, origin choice 2, hex
Te1 2c (1/3,2/3,1/4), Co1 2b (0,0,1/4), Co2 2d (1/3,2/3,3/4), O1 12i (x,y,z), x=-0.35090, y=-0.02250, z= 0.34540, Na1 12i (x,y,z)
Include displacive O, magnetic Co distortions
k point: M, k12 (1/2,0,0)

Choose an IR and OPD (optional):

IR: mM2, mk12t2 OPD:

- Select the IR mM2

ISODISTORT: order parameter direction

Space Group: 182 P6₃2 D6-6, Lattice parameters: a= 5.25880, b= 5.25880, c= 11.16980, alpha= 90.00000, beta= 90.00000, gamma= 120.00000
Default space-group preferences: monoclinic axes a(b)c, monoclinic cell choice 1, orthorhombic axes abc, origin choice 2, hexagonal axes, SSG st
Te1 2c (1/3,2/3,1/4), Co1 2b (0,0,1/4), Co2 2d (1/3,2/3,3/4), O1 12i (x,y,z), x=-0.35090, y=-0.02250, z= 0.34540, Na1 12i (x,y,z), x= 0.43000, y=-0.4
Include displacive O, magnetic Co distortions
k point: M, k12 (1/2,0,0)
IR: mM2, mk12t2

Finish selecting the distortion mode by choosing an order parameter direction

- ☒ P1 (a;0;0) 19.29 P2_12_12_1.1'_C[C222_1], basis={{(2,1,0),(0,1,0),(0,0,1)}, origin=(1/2,1/4,1/4), s=2, i=6, k-active= (1/2,0,0)
- ☐ P2 (a;a;0) 20.36 C222_1.1'_a[P222_1], basis={{(2,2,0),(2,2,0),(0,0,1)}, origin=(1,0,0), s=4, i=12, k-active= (1/2,0,0),(0,1/2,0)
- ☐ P3 (a;a;a) 182.183 P6_32'2', basis={{(0,-2,0),(2,2,0),(0,0,1)}, origin=(0,0,0), s=4, i=8, k-active= (1/2,0,0),(0,1/2,0),(1/2,1/2,0)
- ☐ C1 (a;b;0) 4.10 P2_1.1'_a[P2_1], basis={{(2,2,0),(0,0,-1),(-2,0,0)}, origin=(0,0,0), s=4, i=24, k-active= (1/2,0,0),(0,1/2,0)
- ☐ C2 (a;b;a) 20.33 C2'2'2_1, basis={{(2,0,0),(2,4,0),(0,0,1)}, origin=(0,0,0), s=4, i=24, k-active= (1/2,0,0),(0,1/2,0),(1/2,1/2,0)
- ☐ S1 (a;b;c) 4.7 P2_1.1, basis={{(-2,0,0),(0,0,-1),(0,-2,0)}, origin=(0,0,0), s=4, i=48, k-active= (1/2,0,0),(0,1/2,0),(1/2,1/2,0)

Single-k model

Triple-k model

- Save the 3k model into FullProf PCR

see the provided file “NCTO_3k_Isodistort.pcr”

ISODISTORT: distortion

Space Group: 182 P6₃2 D6-6, Lattice parameters: a= 5.25880, b= 5.25880, c= 11.16980, alpha= 90.00000, beta= 90.00000, gamma= 120.00000
 Default space-group preferences: monoclinic axes a(b)c, monoclinic cell choice 1, orthorhombic axes abc, origin choice 2, hexagonal axes, SSG standard setting
 Te1 2c (1/3,2/3,1/4), Co1 2b (0,0,1/4), Co2 2d (1/3,2/3,3/4), O1 12i (x,y,z), x=-0.35090, y=-0.02250, z= 0.34540, Na1 12i (x,y,z), x= 0.43000, y=-0.40600, z=-0.07700, occ= 0.25800, Na3 2a (0,0,0), occ= 0.38000
 Include displacive O, magnetic Co distortions
 k point: M, k12 (1/2,0,0)
 IR: mM2, mk12t2
 P3 (a,a,a) 182.183 P6₃2', basis={ (0,-2,0), (2,2,0), (0,0,1) }, origin=(0,0,0), s=4, i=8, k-active= (1/2,0,0), (0,1/2,0), (1/2,1/2,0)
 Lattice parameters of undistorted supercell: a=10.51760, b=10.51760, c=11.16980, alpha=90.00000, beta=90.00000, gamma=120.00000

Interactive viewer ☐ Save interactive distortion ☐ Save interactive diffraction ☐ CIF file ☐ Distortion file ☐ Domains ☐ Primary order parameters ☐
☒ FULLPROF.pcr ☐ IR matrices ☐ Subgroup tree ☐ OK
 Enter mode and strain amplitudes:

P6₃2'[1/2,0,0]mM2 (a,a,a) 182.183 P6₃2', basis={ (0,-2,0), (2,2,0), (0,0,1) }, origin=(0,0,0), s=4, i=8, k-active= (1/2,0,0), (0,1/2,0), (1/2,1/2,0)

2 [Co1:b:maj]A2(a)

2 [Co1:b:maj]E(a)

2 [Co2:d:maj]A2(a)

2 [Co2:d:maj]E(a)

The PCR from Isodistort has slightly different settings in the experimental input (wavelength, background points, etc). It is recommended to copy that front section from the previous PCR, made with mcif2pcr tool, and ensure that the **Job** to “1” (for Rietveld fitting) and “**NCY**” to nonzero.

The B-factors also needs to be checked (the program puts some default values).

File	Edit	View
mModes 12		
! Nm	Atm	Irrep
1	Co1_1	mM2
1	Co1_2	mM2
2	Co1_1	mM2
2	Co1_2	mM2
3	Co2_1	mM2
3	Co2_2	mM2
4	Co2_1	mM2
4	Co2_2	mM2
5	Co1_1	mGM2
5	Co1_2	mGM2
6	Co2_1	mGM2
6	Co2_2	mGM2
! Amplitudes of Symmetry Modes		
A_MODES	12	2
Max_Amplitude	0.3000	
A1_GM1	0.000000	0.000000
A2_GM1	0.000000	0.000000
A3_GM1	0.000000	0.000000
A4_M1	0.000000	0.000000
A5_M1	0.000000	0.000000
A6_M1	0.000000	0.000000
A7_M1	0.000000	0.000000
A8_M1	0.000000	0.000000
A9_M1	0.000000	0.000000
A10_M1	0.000000	0.000000
A11_M1	0.000000	0.000000
A12_M1	0.000000	0.000000
! Amplitudes of Magnetic Symmetry Modes		
MA_MODES	6	
A13_mM2	1.414690	11.000000
A14_mM2	5.659220	21.000000
A15_mM2	1.414690	11.000000
A16_mM2	-5.659220	-21.000000
A17_mGM2	0.000000	0.000000
A18_mGM2	0.000000	0.000000
!-----> Profile Parameters for Pattern # 1 -----> Phase # 1		
! Scale	Shape1	Bov
0.2499923	0.00000	0.00000
31.00000	0.000	0.000
! U	V	W
0.176020	-0.197809	0.091458
0.00	0.00	0.00
! a	b	c
10.517600	10.517600	11.169799
0.00000	0.00000	0.00000
! alpha	beta	gamma
90.000000	90.000000	120.000000
0.00000	0.00000	0.00000
# Cell Info		
#box	-0.15 1.15	-0.15 1.15
Size-Model	0	0
GauSiz	0.000000	0.000000
LorSiz	0.000000	0.000000
Strain-Model	0	0
Str1	0.00000	0.00000
Str2	0.00000	0.00000
Str3	0.00000	0.00000
Str4	0.00000	0.00000
Str5	0.00000	0.00000
Str6	0.00000	0.00000
Str7	0.00000	0.00000
Str8	0.00000	0.00000
Str9	0.00000	0.00000
Str10	0.00000	0.00000
Str11	0.00000	0.00000
Str12	0.00000	0.00000
Str13	0.00000	0.00000
Str14	0.00000	0.00000
Str15	0.00000	0.00000
Str16	0.00000	0.00000
Str17	0.00000	0.00000
Str18	0.00000	0.00000
Str19	0.00000	0.00000
Str20	0.00000	0.00000
Str21	0.00000	0.00000
Str22	0.00000	0.00000
Str23	0.00000	0.00000
Str24	0.00000	0.00000
Str25	0.00000	0.00000
Str26	0.00000	0.00000
Str27	0.00000	0.00000
Str28	0.00000	0.00000
Str29	0.00000	0.00000
Str30	0.00000	0.00000
Str31	0.00000	0.00000
Str32	0.00000	0.00000
Str33	0.00000	0.00000
Str34	0.00000	0.00000
Str35	0.00000	0.00000
Str36	0.00000	0.00000
Str37	0.00000	0.00000
Str38	0.00000	0.00000
Str39	0.00000	0.00000
Str40	0.00000	0.00000
Str41	0.00000	0.00000
Str42	0.00000	0.00000
Str43	0.00000	0.00000
Str44	0.00000	0.00000
Str45	0.00000	0.00000
Str46	0.00000	0.00000
Str47	0.00000	0.00000
Str48	0.00000	0.00000
Str49	0.00000	0.00000
Str50	0.00000	0.00000
Str51	0.00000	0.00000
Str52	0.00000	0.00000
Str53	0.00000	0.00000
Str54	0.00000	0.00000
Str55	0.00000	0.00000
Str56	0.00000	0.00000
Str57	0.00000	0.00000
Str58	0.00000	0.00000
Str59	0.00000	0.00000
Str60	0.00000	0.00000
Str61	0.00000	0.00000
Str62	0.00000	0.00000
Str63	0.00000	0.00000
Str64	0.00000	0.00000
Str65	0.00000	0.00000
Str66	0.00000	0.00000
Str67	0.00000	0.00000
Str68	0.00000	0.00000
Str69	0.00000	0.00000
Str70	0.00000	0.00000
Str71	0.00000	0.00000
Str72	0.00000	0.00000
Str73	0.00000	0.00000
Str74	0.00000	0.00000
Str75	0.00000	0.00000
Str76	0.00000	0.00000
Str77	0.00000	0.00000
Str78	0.00000	0.00000
Str79	0.00000	0.00000
Str80	0.00000	0.00000
Str81	0.00000	0.00000
Str82	0.00000	0.00000
Str83	0.00000	0.00000
Str84	0.00000	0.00000
Str85	0.00000	0.00000
Str86	0.00000	0.00000
Str87	0.00000	0.00000
Str88	0.00000	0.00000
Str89	0.00000	0.00000
Str90	0.00000	0.00000
Str91	0.00000	0.00000
Str92	0.00000	0.00000
Str93	0.00000	0.00000
Str94	0.00000	0.00000
Str95	0.00000	0.00000
Str96	0.00000	0.00000
Str97	0.00000	0.00000
Str98	0.00000	0.00000
Str99	0.00000	0.00000
Str100	0.00000	0.00000

Refine the amplitudes of magnetic modes and the scale factor

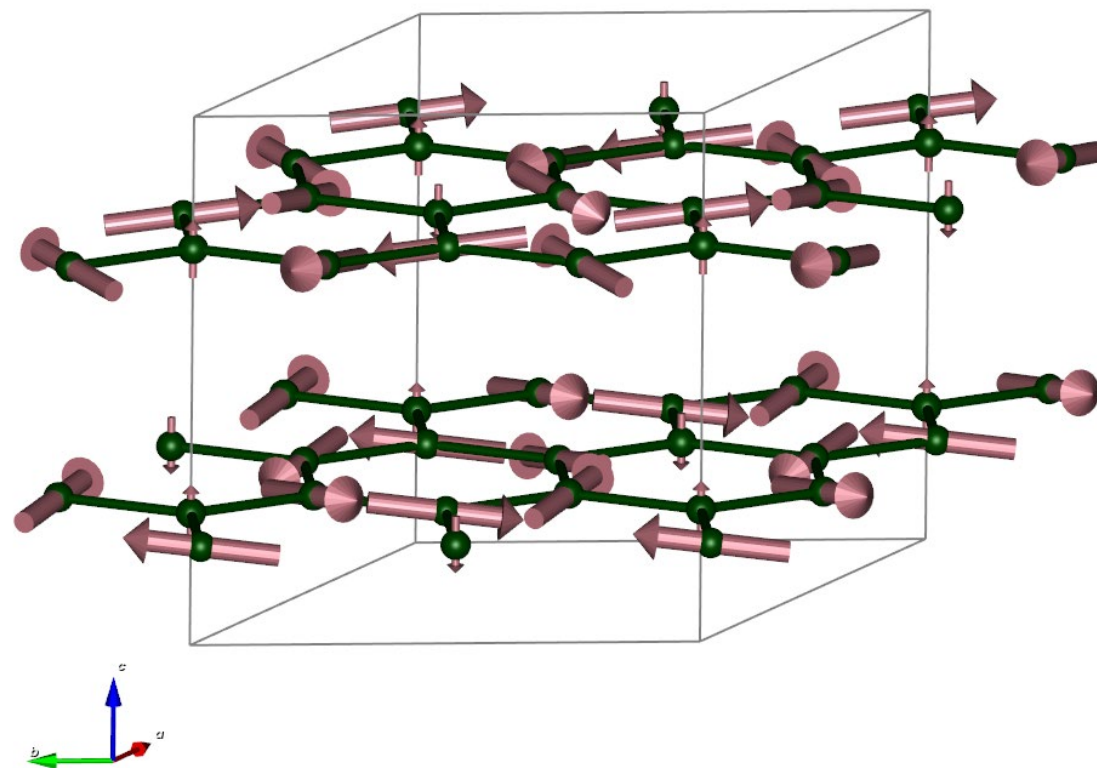
- Get the refined moment value from *.sum or *.out output files

		X	Y	Z	Biso	Occ	
Atom	Te1_1	TE	0.83333	0.66667	0.25000	0.00000	0.50000
Atom	Te1_2	TE	0.33333	0.66667	0.25000	0.00000	0.16667
Atom	Co1_1	MC02	0.00000	0.00000	0.25000	0.00000	0.16667
Moment(mx,my,mz):			0.00000	0.00000	0.87(3)		
Atom	Co1_2	MC02	0.50000	0.00000	0.25000	0.00000	0.50000
Moment(mx,my,mz):			-2.309(5)	0.00000	-0.289(8)		
Atom	Co2_1	MC02	0.16667	0.33333	0.25000	0.00000	0.50000
Moment(mx,my,mz):			2.309(5)	0.00000	0.289(8)		
Atom	Co2_2	MC02	0.33333	0.66667	0.75000	0.00000	0.16667
Moment(mx,my,mz):			0.00000	0.00000	-0.87(3)		
Atom	O1_1	O	0.83580	0.82455	0.34540	0.00000	1.00000
Atom	O1_2	O	0.83580	0.32455	0.34540	0.00000	1.00000
Atom	O1_3	O	0.33580	0.82455	0.34540	0.00000	1.00000

- Or from the created FullProf Studio file
NCTO_3k_isodistort_1_Irrep_M1.fst

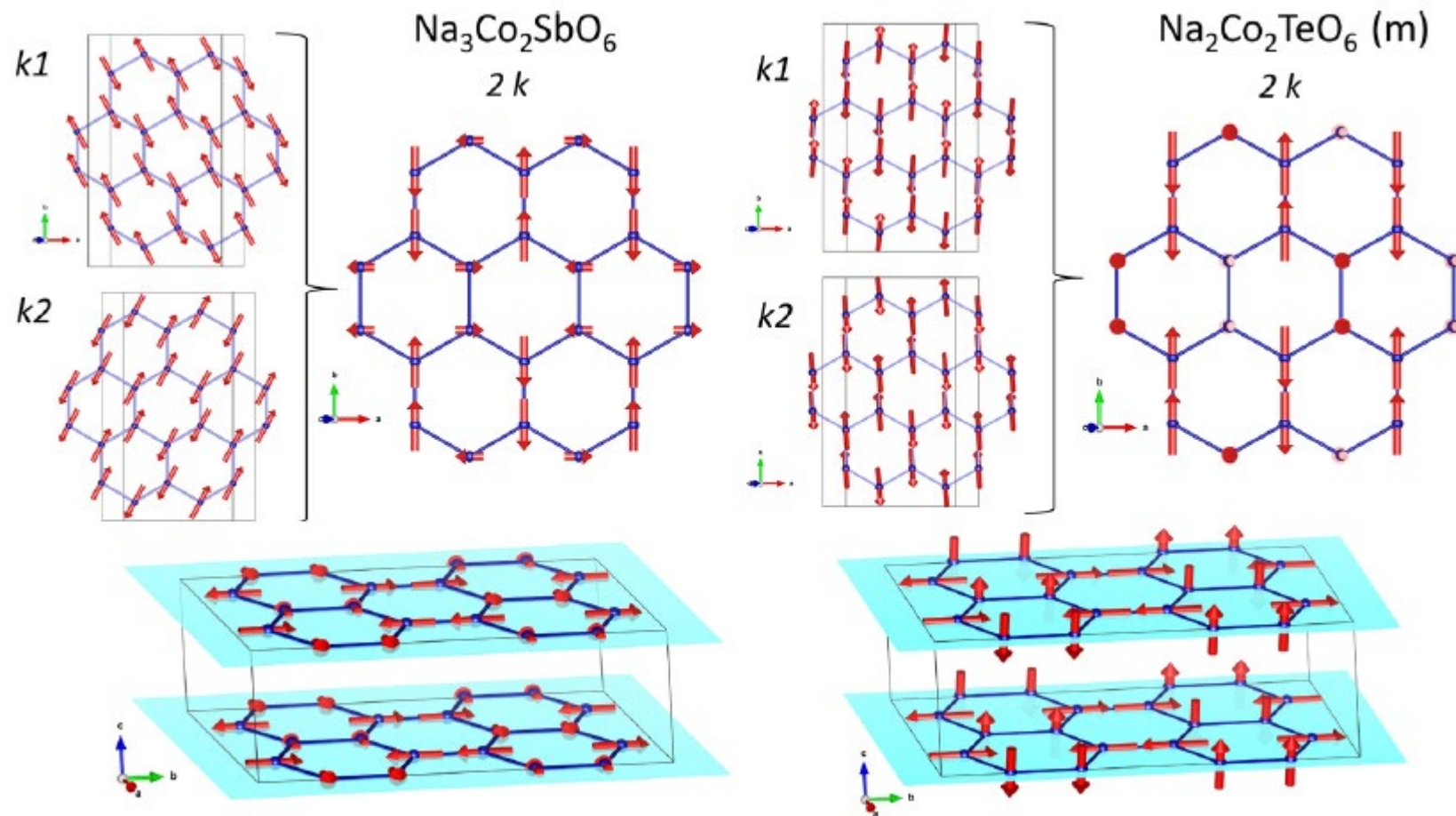
MATOMP	V, U, W, 0, 0							
MATOMP	Co1_1	Co	0.00000	0.00000	0.25000	SCALE 1.0	GROUP	
SKP	1 1		0.00000	0.00000	0.86594	0.00000	0.00000	0.00000
MATOMP	Co1_2	Co	0.50000	0.00000	0.25000	SCALE 1.0	GROUP	
SKP	1 1		-2.30943	0.00000	-0.28917	0.00000	0.00000	0.00000
MATOMP	Co2_1	Co	0.16667	0.33333	0.25000	SCALE 1.0	GROUP	
SKP	1 1		2.30943	0.00000	0.28917	0.00000	0.00000	0.00000
MATOMP	Co2_2	Co	0.33333	0.66667	0.75000	SCALE 1.0	GROUP	
SKP	1 1		0.00000	0.00000	-0.86594	0.00000	0.00000	0.00000

FullProf Studio created picture



Optional homework:

- load the single-k file of $\text{Na}_2\text{Co}_2\text{SbO}_6$ from MagnData (entry# [1.788](#)) and create the 2k magnetic structure (see result in the entry # [2.116](#))



V. O Garlea, C. Sarkis, *Acta Cryst. B* (2025) 81 11 - 27

DOI: [10.1107/S2052520624009831](https://doi.org/10.1107/S2052520624009831)