Introduction to

Mag2Pol

A user-friendly software for the analysis of powder and single-crystal diffraction data

Navid Qureshi

Outline

Content of the presentation

Why a new software?
Reasons and motivations for development

About Mag2Pol
Technical details, evolution, basic features

Demonstration
General features, q-vector finder, MSGs, MSSGs

Conclusions

Why a new software?

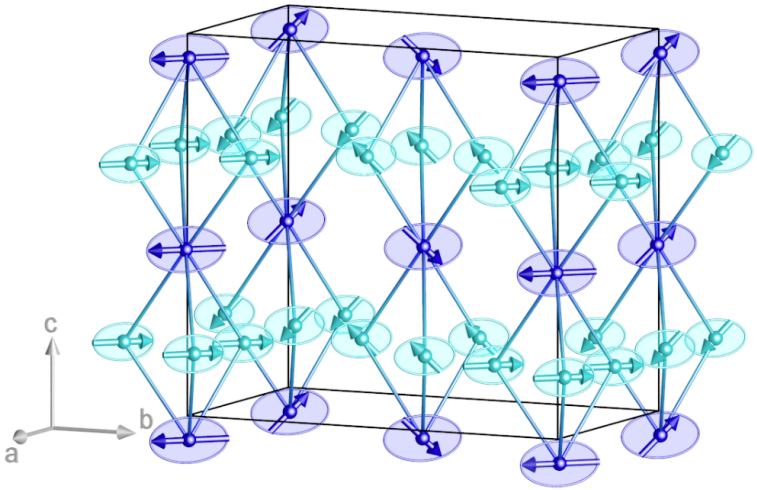
Scientific reason

October 2015: D3/Cryopad experiment on $CaBaCo_3FeO_7$

- complex magnetic structure
- polarization matrices not easily interpretable
- presence of magnetic domains and structural twins
- necessity to co-refine unpolarized and SNP data

On the market:

- muFit
- CrysFML routine (never tested)



Qureshi et al. (2018) *Phys. Rev. B* **97** 064404

Result: A software that brings you from a **mag**netic structure **to** a **pol**arization matrix

Why a new software?

Workflow reason

ARRNGE	averaging, statistics	DATARED
AVEXAR	absorption/extinction correction	DATAP
SFLSQ	least-squares refinement	FP2K
MAG3D	structure visualisation	FP STUDIO

Why a new software?

User-friendliness reason

```
N CaBaFe4O7
C   6.3546 10.9763 10.3584  90.000000  90.000000  90.000000
Z-------------------------------------------------------------
Z symmetry operators
S        X,          Y,          Z
S       -X,         -Y,      1/2+Z
S   1/2-X,      1/2+Y,          Z
S   1/2+X,      1/2-Y,      1/2+Z
Z-------------------------------------------------------------
Z atomic positions
A Ca    -0.00158   0.66696   0.86563   0.56195
A Ba    -0.00932   0.66602   0.49505   1.20190
A Fe1   -0.00310  -0.00046   0.92866   0.41705
A Fe2   -0.00628   0.17924   0.67825   1.23871
A Fe3    0.28075   0.09469   0.17438   0.80456
A Fe4    0.25630   0.91606   0.68004   1.20547
A O1     0.00689   0.00181   0.24446   0.80246
A O2    -0.99518   0.49230   0.22544   4.21763
A O3     0.78042   0.26039   0.77335   1.79120
A O4     0.73241   0.75678   0.21200   0.87593
A O5    -0.05401   0.15473   0.49265   0.95823
A O6     0.20414   0.10446  -0.00261   1.22739
A O7     0.25772   0.94950   0.50260   1.27410
Z-------------------------------------------------------------
Z nuclear scattering factors
F Ca      1   0.47000
F Ba      1   0.50700
F Fe      1   0.94500
F O       1   0.58030
Z-------------------------------------------------------------
Z form factor table
ZF Fe 2 0.0263 34.9597 0.3668 15.9435 0.6188 5.5935 -0.0119
ZF Fe 4 1.6490 16.5593 1.9064  6.1325 0.5206 2.1370  0.0035
F FeM 3  0.00   1.0000  0.05   0.9798  0.10   0.9230  0.15   0.8390  0.20   0.73
F FeM 3  0.25   0.6360  0.30   0.5362  0.40   0.3660  0.50   0.2411  0.60   0.15
F FeM 3  0.70   0.0971  0.80   0.0610  0.90   0.0389  1.00   0.0249  1.10   0.01
F FeM 3  1.20   0.0083  1.30   0.0030  1.40   0.0000  1.50   0.0000  1.60   0.00
```

```
COMM CaBaFe4O7 300K nuclear Pbn21
! Current global Chi2 (Bragg contrib.) =      104.0
! Files => DAT-file: k0220k_Cmc21,  PCR-file: k0_pbn21
!Job Npr Nph Nba Nex Nsc Nor Dum Iwg Ilo Ias Res Ste Nre Cry Uni Cor Opt Aut
   1   0   1   0   0   0   0   0   0   0   1   0   0   0   1   0   0   0   0
!
!Ipr Ppl Ioc Mat Pcr Ls1 Ls2 Ls3 NLI Prf Ins Rpa Sym Hkl Fou Sho Ana
   0   0   1   0   1   0   4   0   0   1  10   0   1   0   0   1   0
!
!NCY  Eps  R_at  R_an  R_pr  R_gl     Thmin       Step       Thmax    PSD    Sent0
 20  0.05  1.00  1.00  1.00  1.00      0.0000   0.050016   159.9500   0.000   0.000
!
!
     4    !Number of refined parameters
!-------------------------------------------------------------------------------
!  Data for PHASE number:   1  ==> Current R_Bragg for Pattern#  1:     8.41
!-------------------------------------------------------------------------------
 phase 1:
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth       ATZ    Nvk Npr More
  13   0   0 0.0 0.0 1.0  10   4  -1   0   0       1626.710   0   5   0
!
P b n 21                  <--Space group symbol
!Nsym Cen Laue MagMat
   4   1   1   1
!
SYMM x,y,z
MSYM u,v,w, 0.0
SYMM -x,-y,z+1/2
MSYM -u,-v,w, 0.0
SYMM -x+1/2,y+1/2,z
MSYM -u,v,w, 0.0
SYMM x+1/2,-y+1/2,z+1/2
MSYM u,-v,w, 0.0
!
```

About Mag2Pol

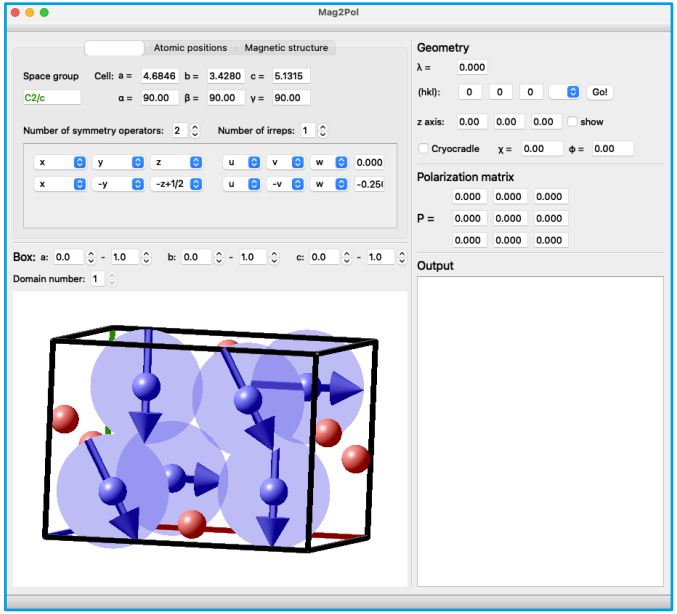
Basic features

- **What is Mag2Pol?** Analysis software for X-ray and (polarized) neutron diffraction data
- **What does it do?** Visualizing and refining nuclear and magnetic structures (+ a lot of useful tools)
- **What kind of data?** Powder patterns, integrated intensities, flipping ratios, polarization matrices
- **What is it written in?** C++ (Qt5, Eigen, QCustomPlot, OpenGL, tinyxml2)
- **Where can I get it?** Download standalone package for Windows, macOS or Linux on www.ill.eu/mag2pol
- **Is there any documentation?** Qureshi, *J. Appl. Cryst.* **52** 175 (2019), up-to-date manual, examples, tutorials, introductory courses

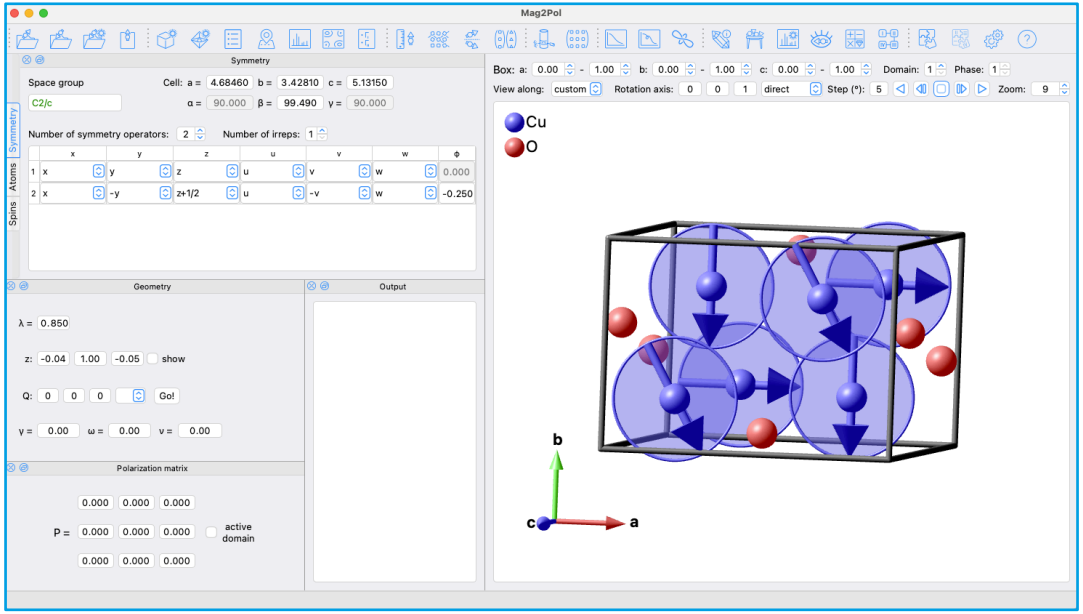
About Mag2Pol

Evolution

First released version 1.3.1 (2018)



Latest version 7.2.2 (2025)



About Mag2Pol

Evolution

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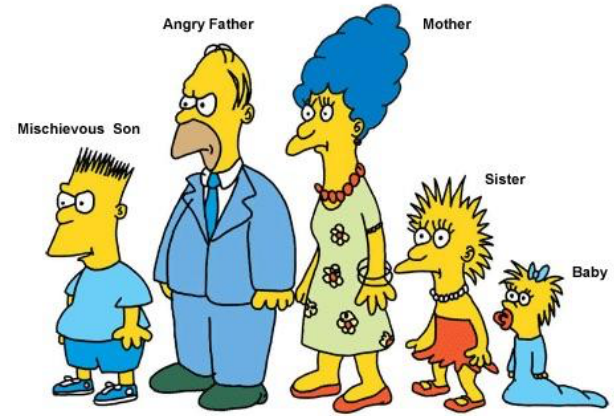

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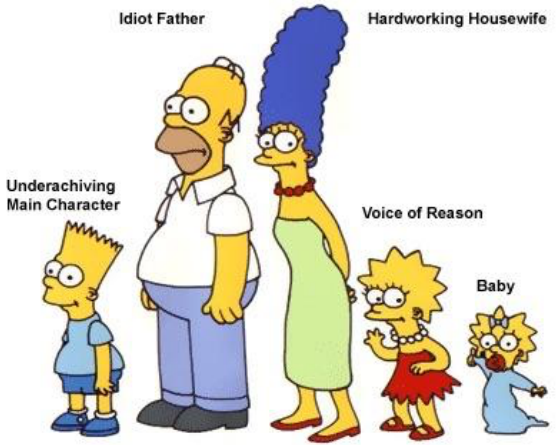
(2025)



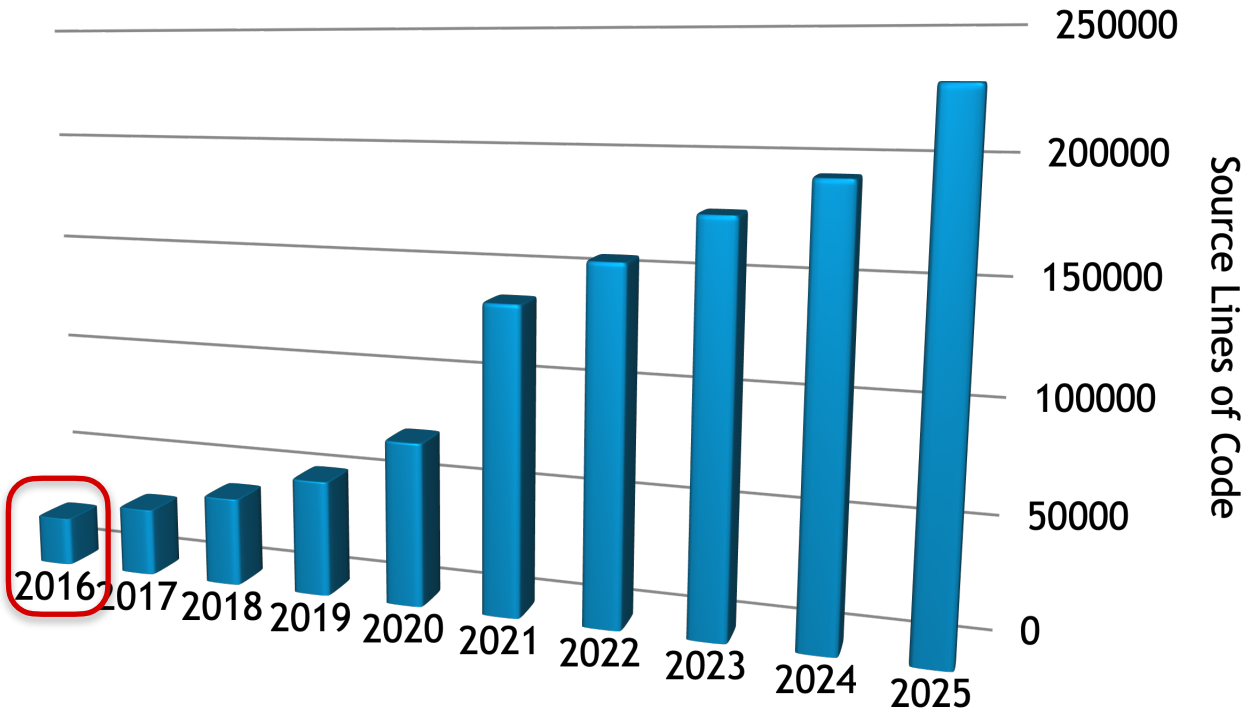
About Mag2Pol

Evolution

MAG2POL

v1.0

- 3D unit cell plot (nuc + mag)
- Space group support
- Calculation of single (hkl)
- Refinement of SNP data
- Magnetic domains
- ^{3}He cell correction

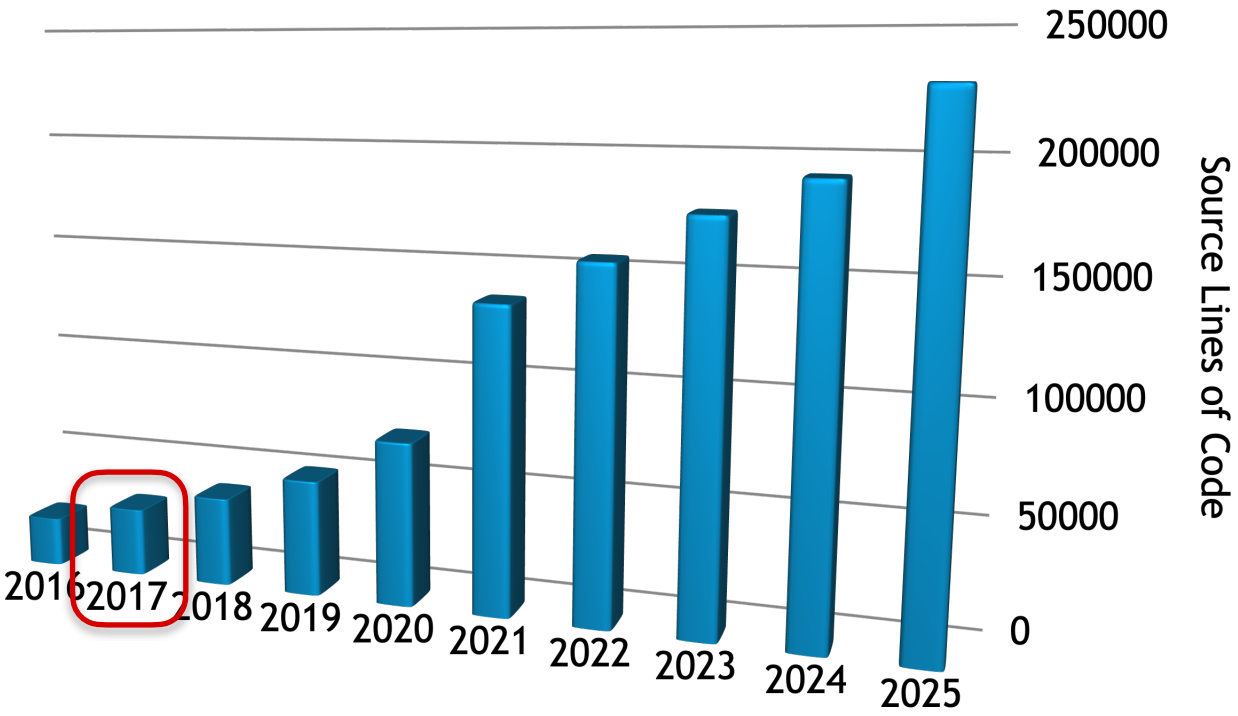


About Mag2Pol

Evolution

v1.0

- Co-refinement of INT and SNP
- Structural twins
- Constraints
- Reflection lists
- Intensity maps and cuts
- Form factor plots
- Multipole expansion

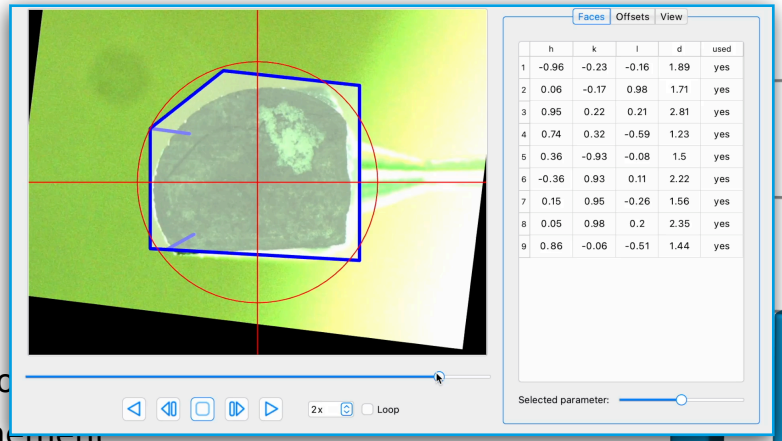


About Mag2Pol

Evolution

MAG2POL

v1.0 - v2.2



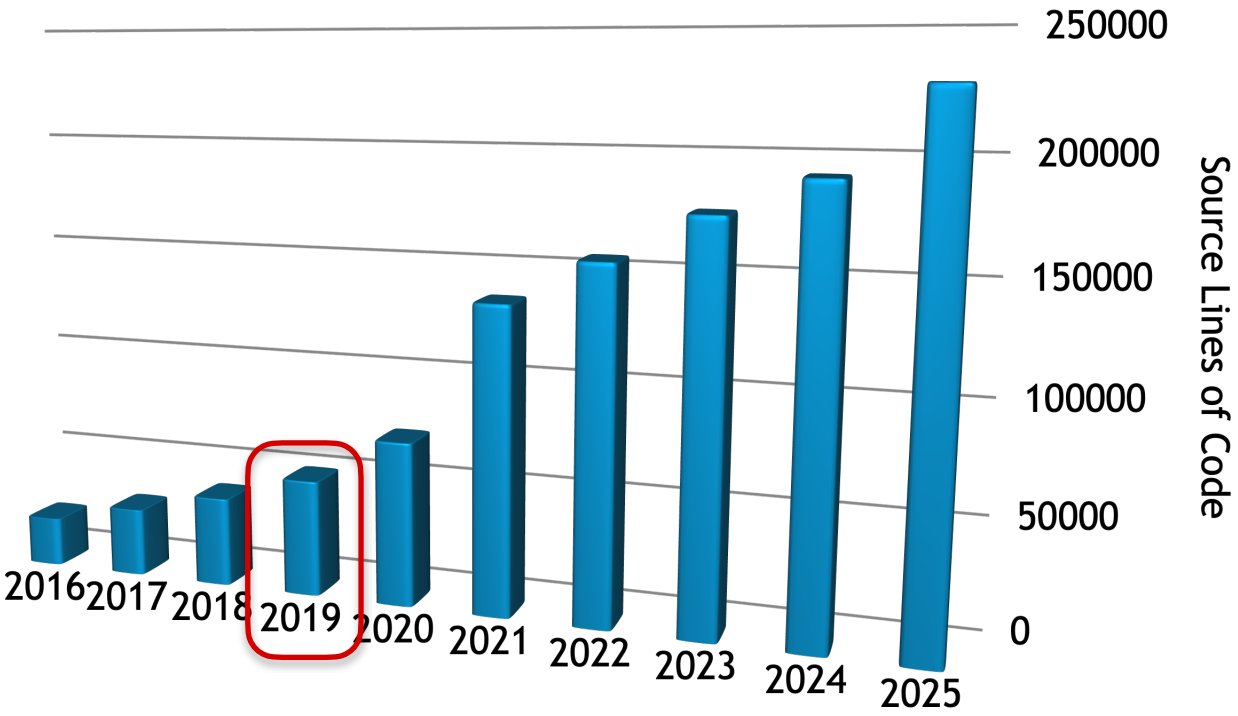
- Cif- and mcif file suppo
- Nuclear structure refinement
- Absorption correction
- Crystal model tool
- Basis vectors
- Anisotropic temperature factors

About Mag2Pol

Evolution

v2.3 - v2.4

- Instrument definitions
- Xml file support
- Isotope support
- X-ray support
- Multiple INT data support
- Distance and angle calculations

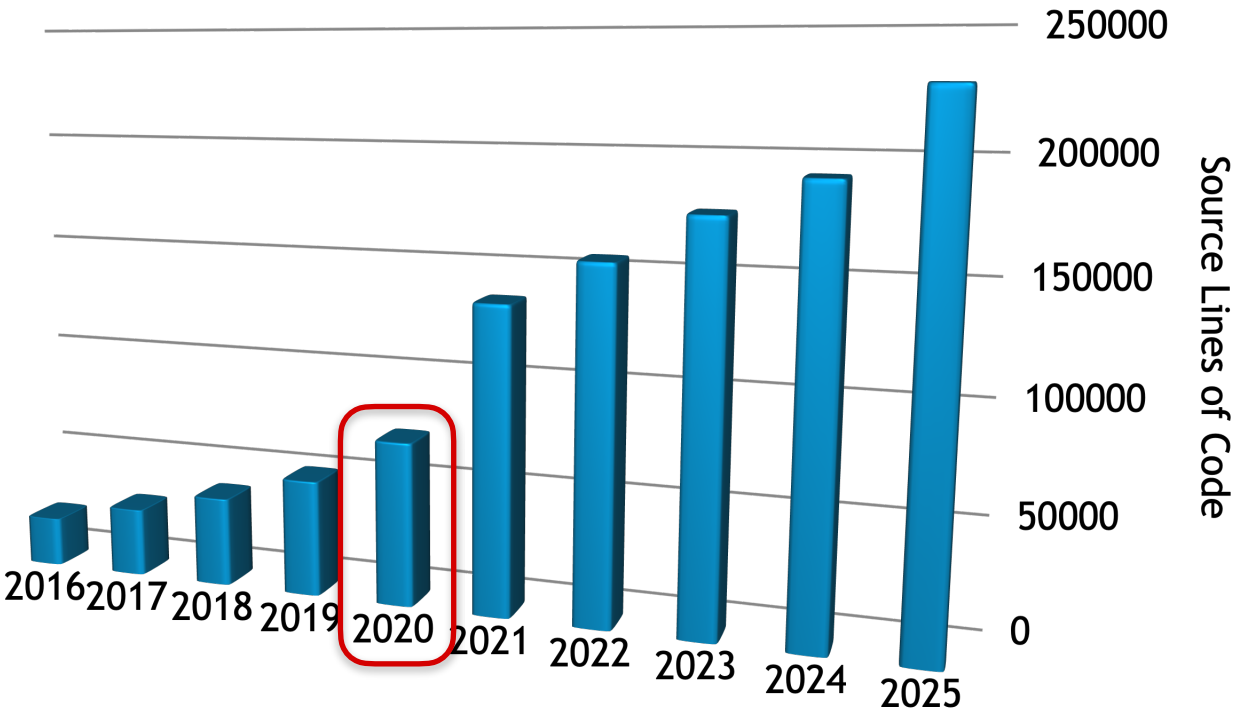


About Mag2Pol

Evolution

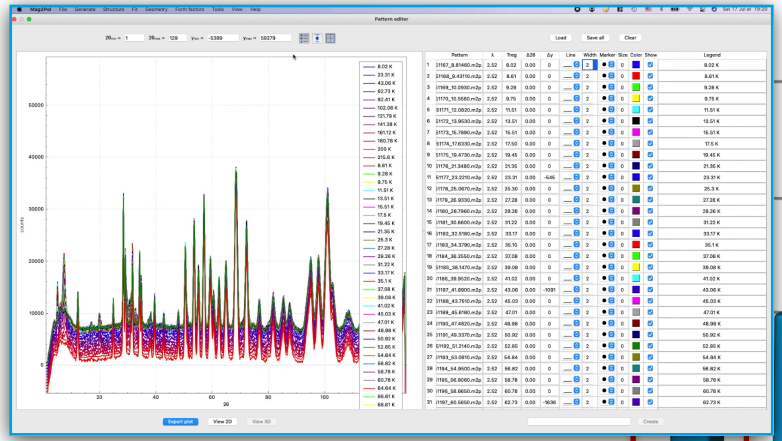
v3.0 - v3.2

- Irreducible calculations
- Powder pattern simulation
- Magnetization density maps
- Multiple phase support
- Schwinger flipping ratios
- Graphics update
- Bonds and polyhedra
- 3D maps



About Mag2Pol

Evolution



v3.3 - v4.3

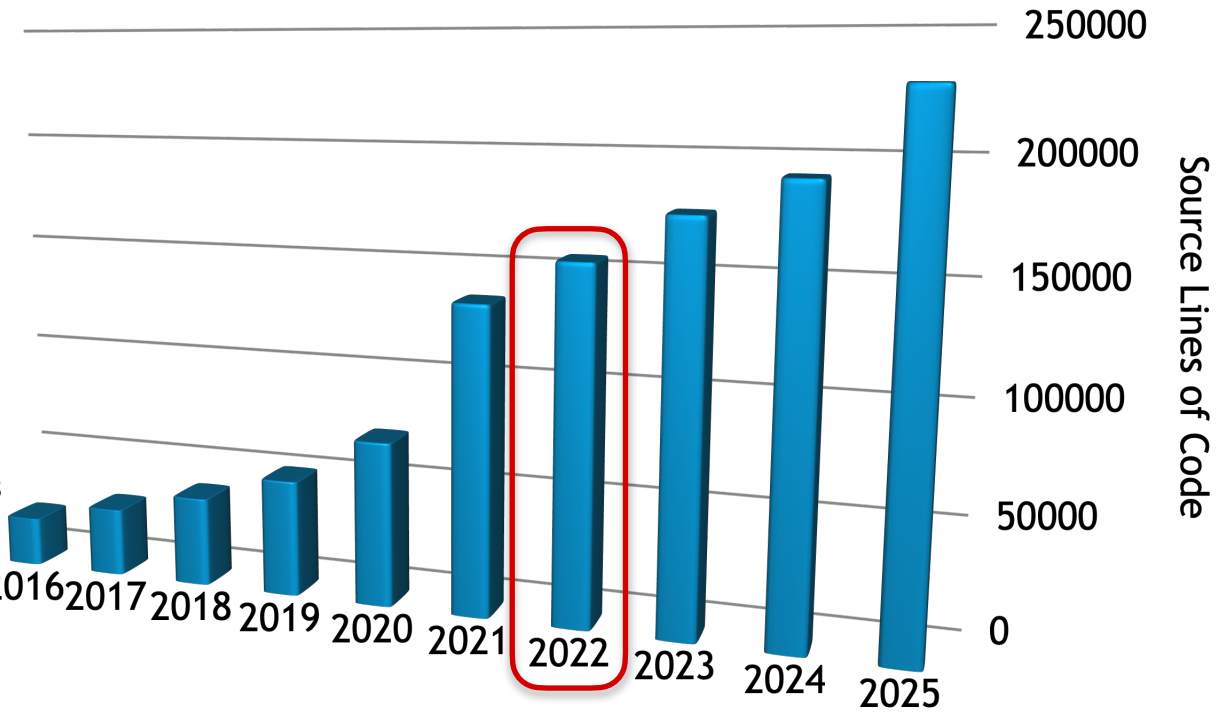
- Spin-correlation tool
- Magnetic PDF
- Multi-q structure plot
- Redesigned app
- Rietveld (batch) refinement
- Pattern plotter (1D, 2D, 3D)
- UB matrix tool
- 3D guides to the eye

About Mag2Pol

Evolution

v4.4 - v5.1

- Customizable toolbar
- TOF Rietveld refinement
- Site symmetry detection for ADPs
- Multi-q and configurational domains
- Magnetic form factor models
- Space group tables, MSGs, MSSGs

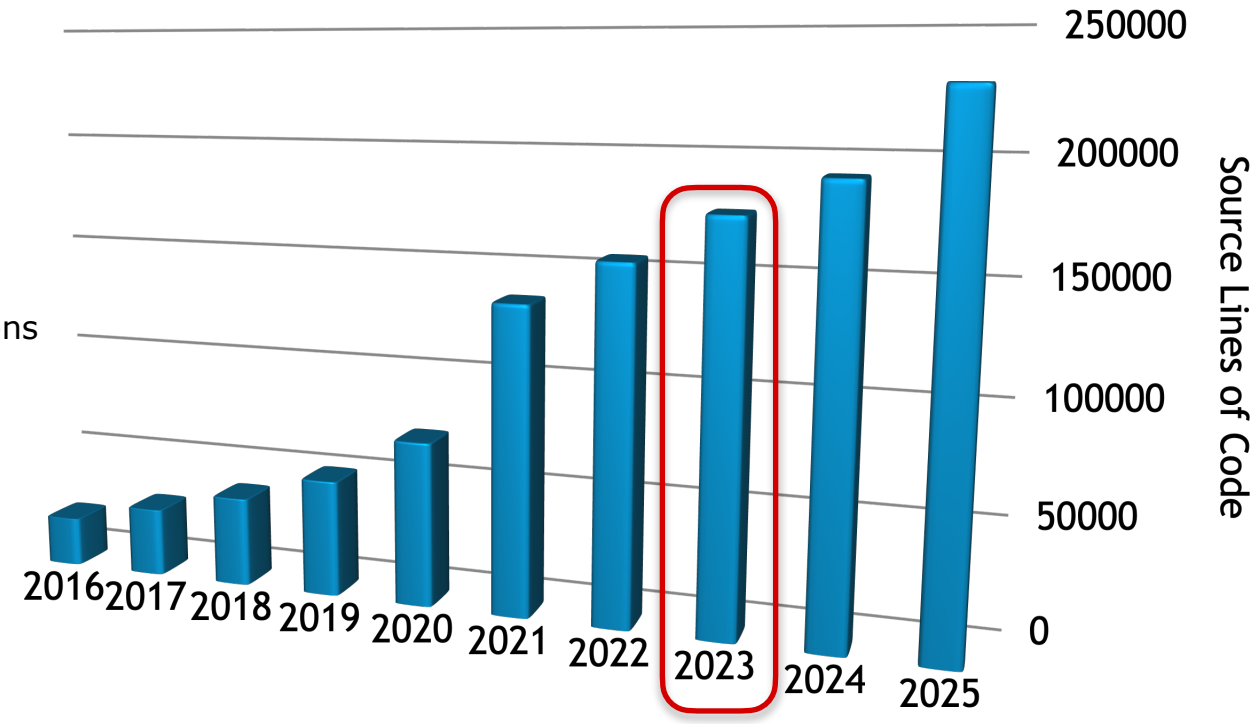


About Mag2Pol

Evolution

v5.2 - v6.0

- Group-to-subgroup transformations
- Interactive pattern simulation
- q-vec and cell finder
- LeBail refinement
- Local susceptibility approach
- Multiple FR or SNP file support
- Crystal calculator tool
- Fit macros

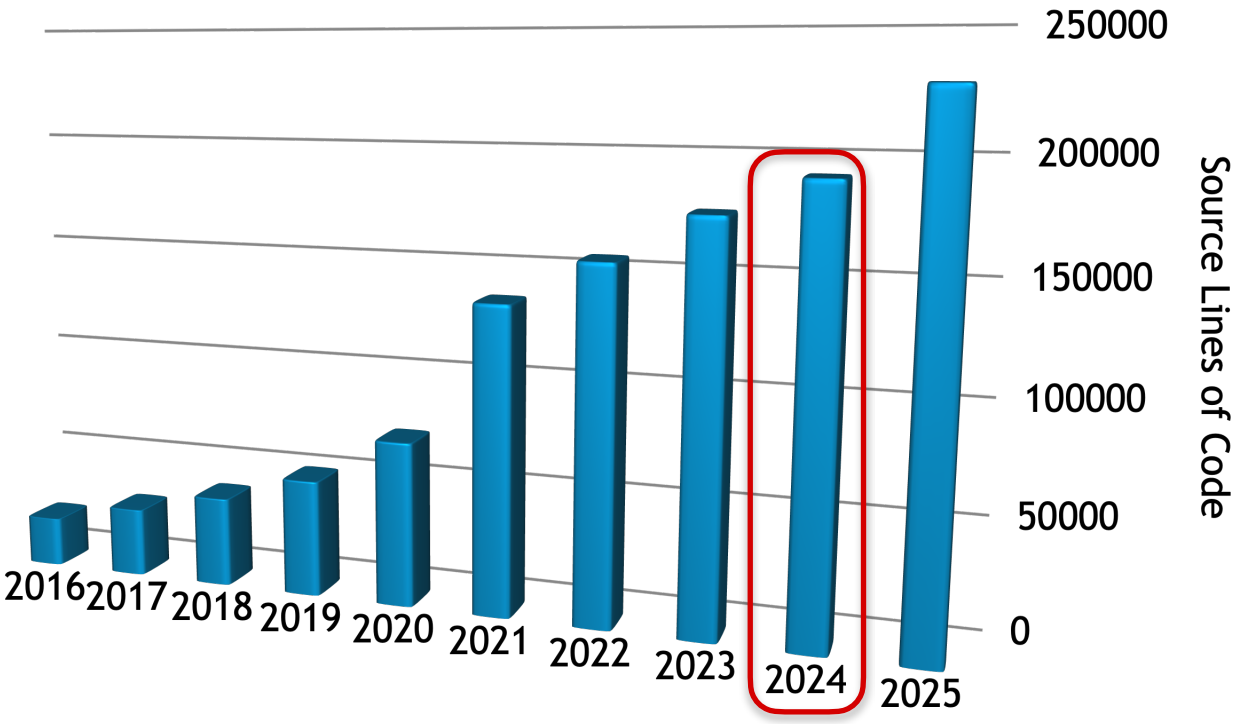


About Mag2Pol

Evolution

v6.1 - v7.0

- Perspective view
- Depth effect
- Cell animation tool
- Rigid bodies
- IRF files
- Microstructure analysis
- Freeform constraints



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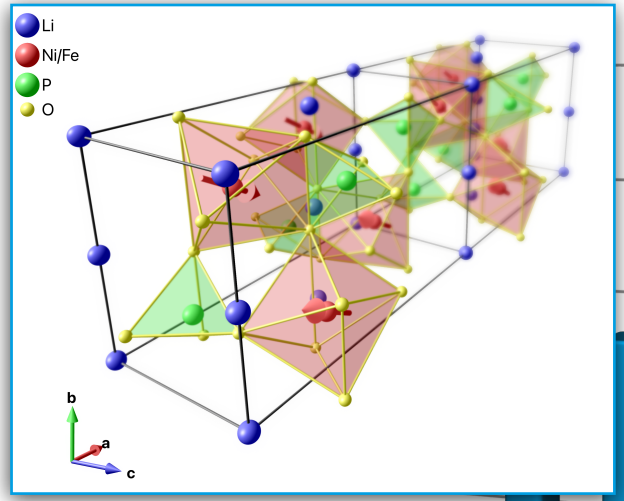

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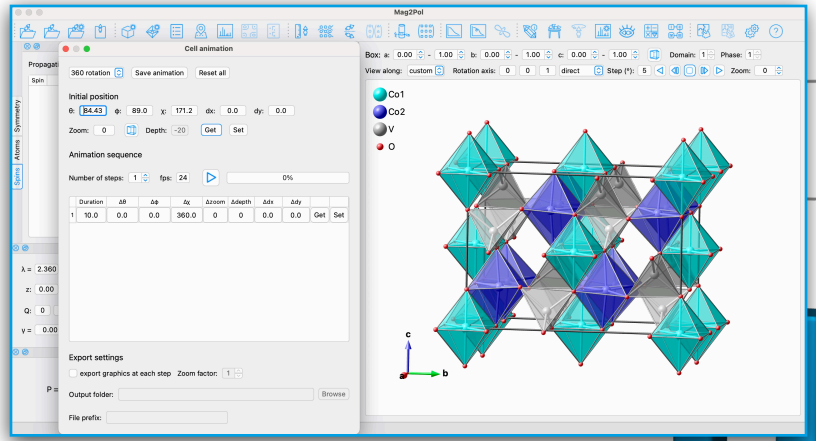

About Mag2Pol

Evolution

v6.1 - v7.0

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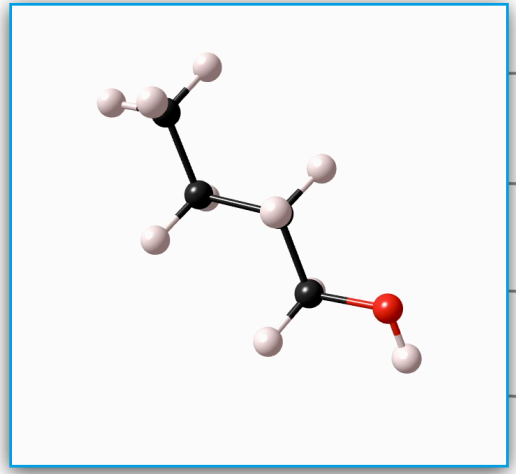
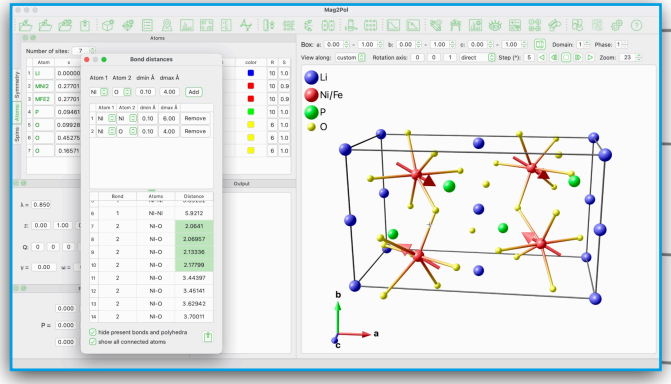


About Mag2Pol

Evolution

v7.1 - v7.2



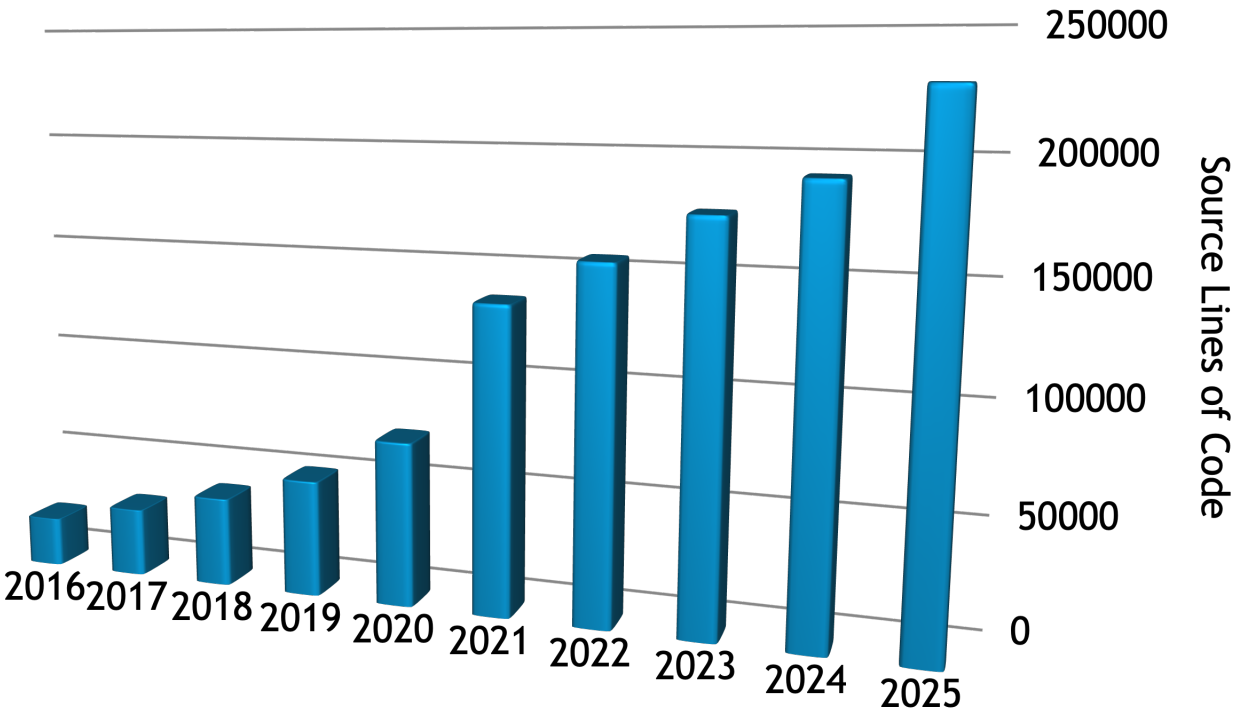
- Bond distance tool
- CDML labels
- Brillouin zone labels
- 3D model export
- Mixed irreps fit macros
- Multipattern batch fit

About Mag2Pol

Evolution

future v8.0

- irreps of the full group
- physically irreducible irreps
- multi-q structures
- TOF single crystal
- twin visualization



About Mag2Pol

Evolution

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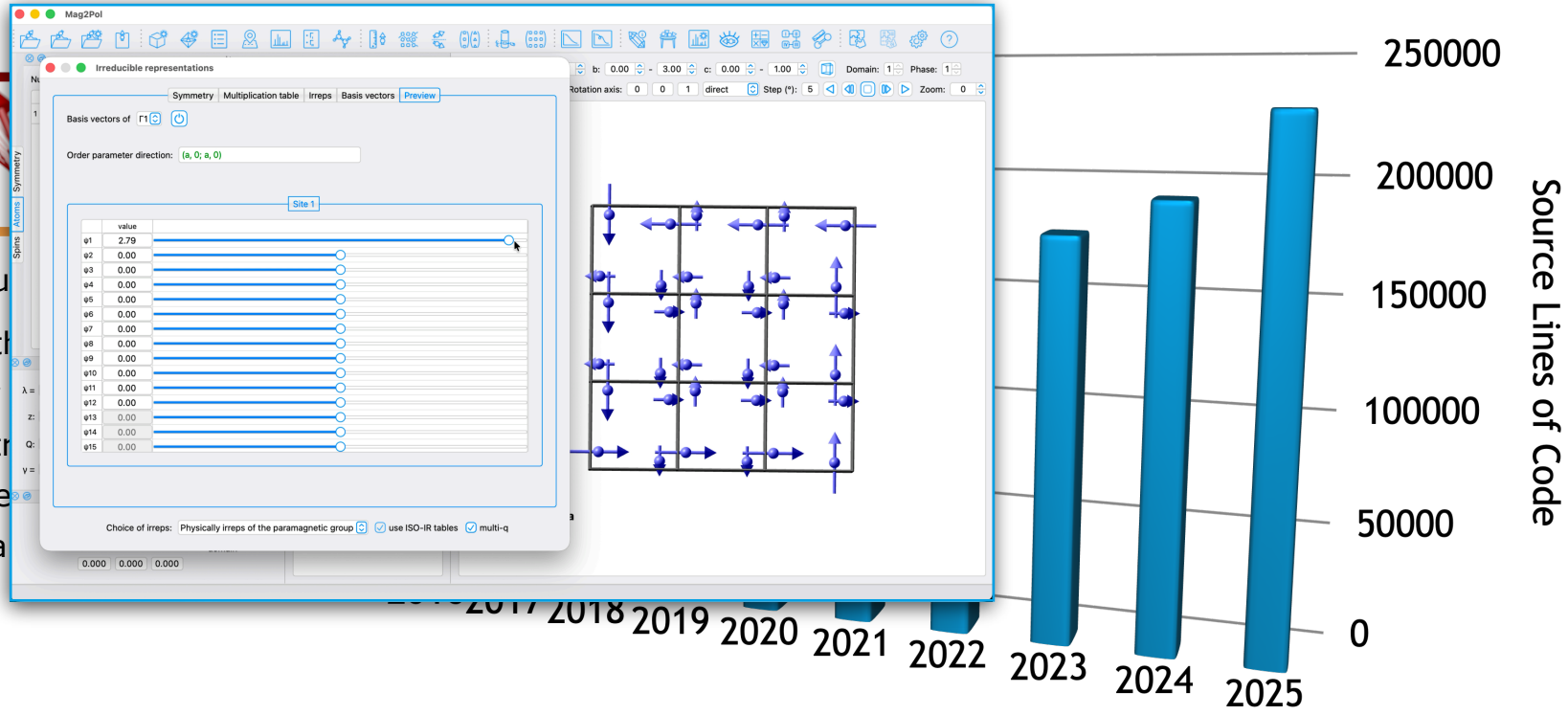
- irreps of th
- physically
- multi-q str
- TOF single
- twin visua

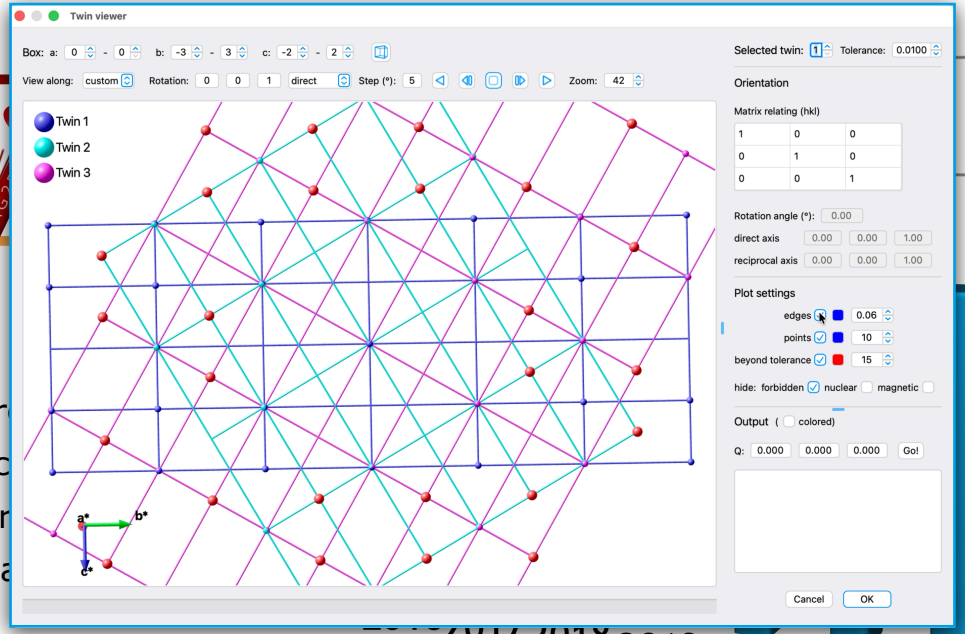


About Mag2Pol

Evolution

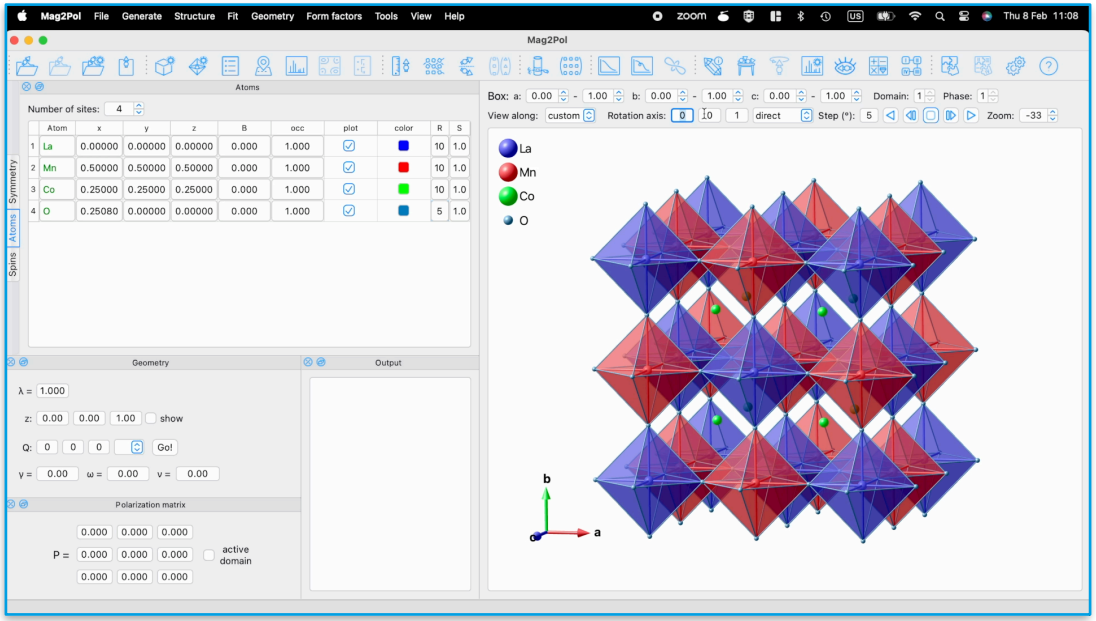
future

- irreps of the
- physically irr
- multi-q struc
- TOF single cr
- twin visualiza



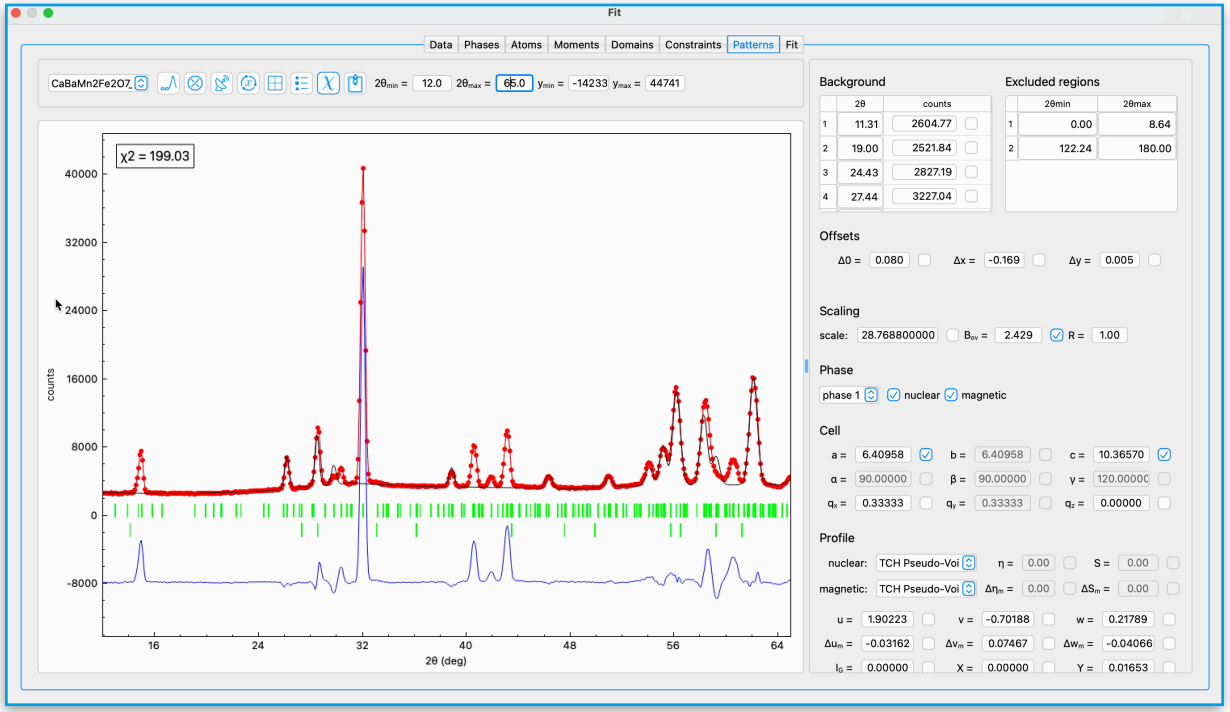
Demonstration

General features



Demonstration

Propagation vector finder



Demonstration

Magnetic space groups

Example: $GdMn_2O_3$, *Pbam* (#55), **q** = (½ 0 0) using MAXMAGN from the BCS (crystal.ehu.es)

Perez-Mato et al., *Annu. Rev. Mater. Res.* **45** 13 (2015)

Maximal magnetic space groups for the parent space group *Pbam* (No. 55) and the propagation vector k = (1/2, 0, 0)

N	Group (BNS)	Transformation matrix	General positions	Properties
1	$P_a ca2_1$ (#29.104) Go to a subgroup	$\begin{pmatrix} 2 & 0 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR
2	$P_b mc2_1$ (#26.72) Go to a subgroup	$\begin{pmatrix} 0 & 2 & 0 & 1/4 \\ 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR
3	$P_c 2/c$ (#13.72) Go to a subgroup	$\begin{pmatrix} 0 & 0 & 2 & 1/2 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR
4	$P_a 2/m$ (#10.47) Go to a subgroup	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR

Demonstration

Magnetic space groups

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Perez-Mato et al., *Annu. Rev. Mater. Res.* **45** 13 (2015)

General positions of the magnetic space group $P_ac a 2_1$ (#29.104) in the basis (2a, b, c; 0, 0, 0) of the parent space group *Pbam* (No. 55)

Transformation matrix:

$$\begin{pmatrix} 1 & 0 & 0 & 1/8 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

Demonstration

Magnetic space groups

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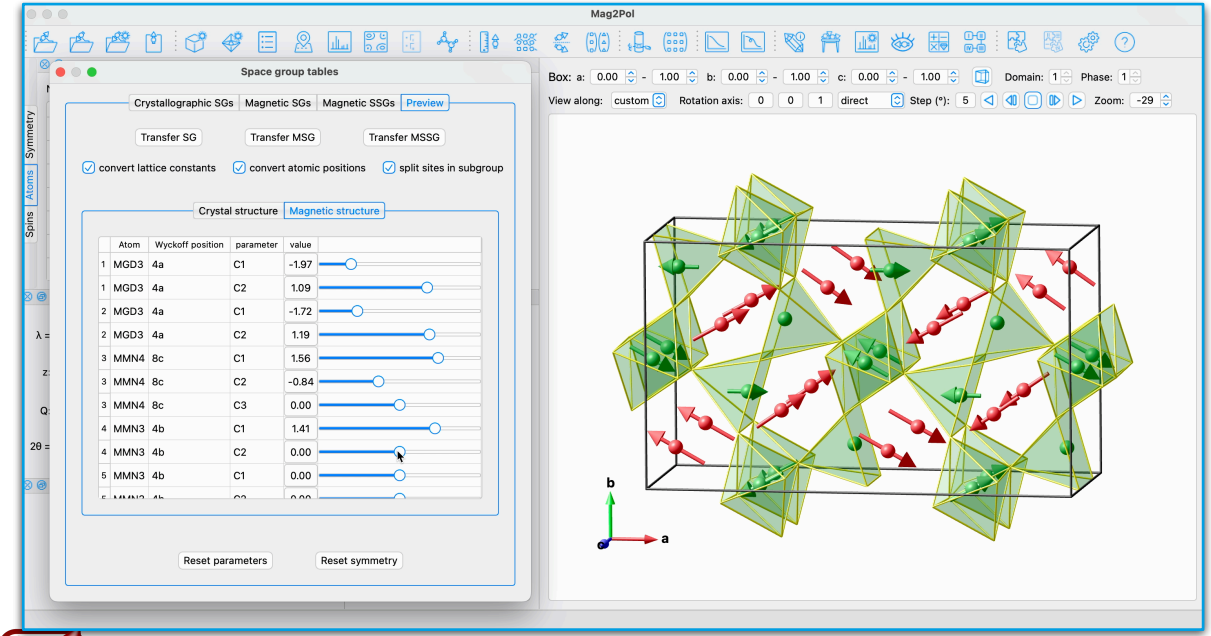


- parent SG transformation
- MSG transformation
- automatic splitting of sites
- test structural/magnetic d.o.f.

Demonstration

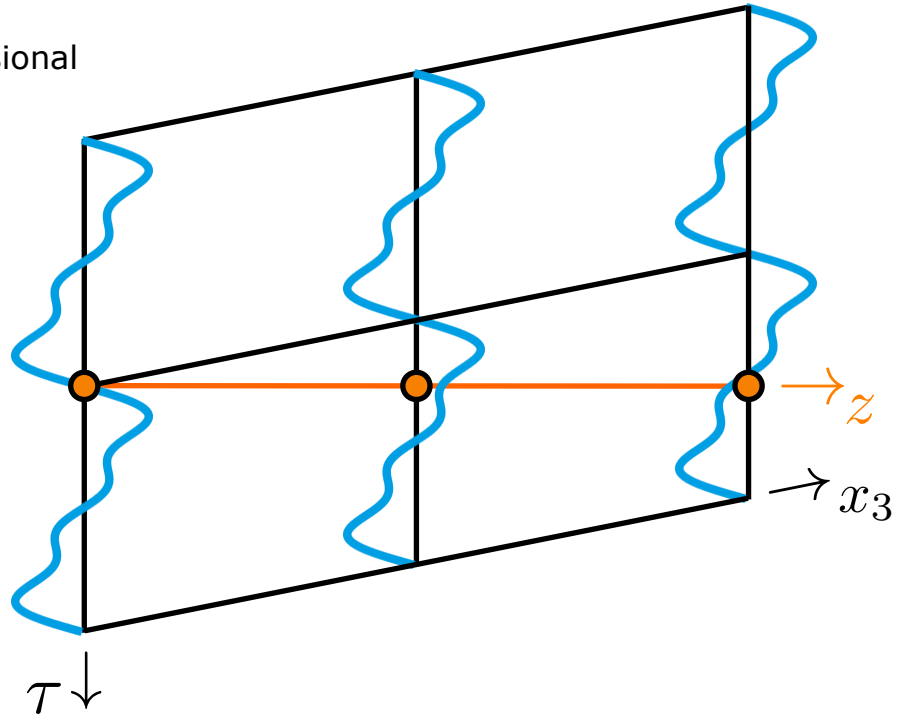
Magnetic superspace groups

Superspace approach: generalization to a higher-dimensional space in order to recover translational symmetry

additional **modulation functions** (atomic positions, magnetic moments, thermal displacement tensor, occupation probability …

Consider atomic modulation with propagation vector along z —> symmetry is recovered by **superspace translation**

There are 9303 (3+1)d, 53756 (3+2)d and 262068 (3+3)d MSSGs Stokes and Campbell, *Acta Cryst.* A**78** 364 (2022)



Demonstration

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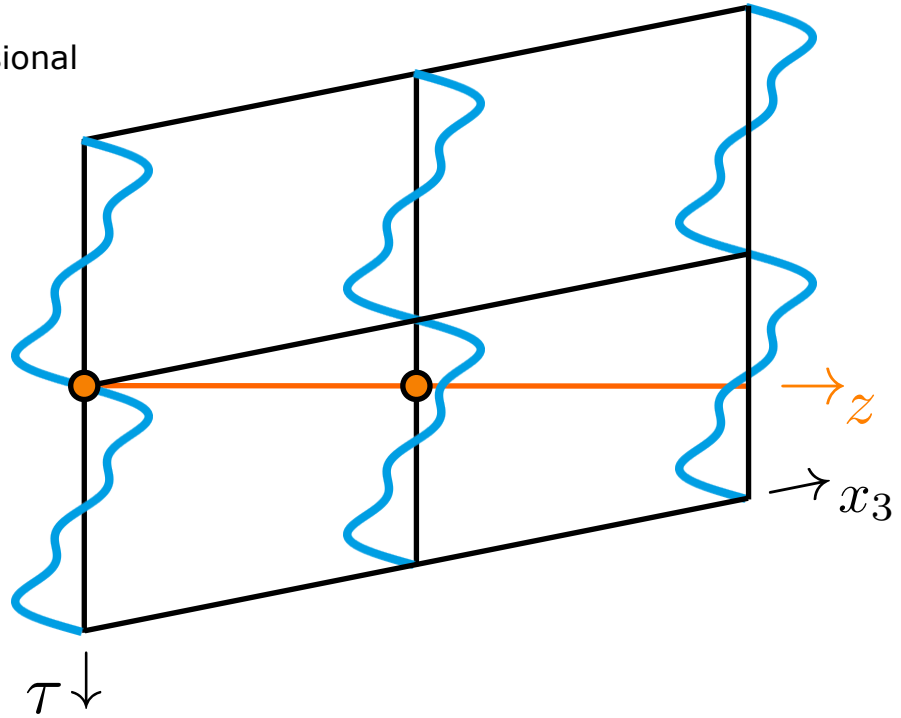


Demonstration

Magnetic superspace groups

In (3+1)d space superspace (= 1 modulation) operators are **4-dimensional**

Seitz notation: $(\mathbf{R}_s, \theta|\mathbf{t}_s)$

$$\begin{pmatrix} x' \\ y' \\ z' \\ \tau' \end{pmatrix} = \begin{pmatrix} R_{11} & R_{12} & R_{13} & 0 \\ R_{21} & R_{22} & R_{23} & 0 \\ R_{31} & R_{32} & R_{33} & 0 \\ H_{R1} & H_{R2} & H_{R3} & R_I \end{pmatrix} \cdot \begin{pmatrix} x \\ y \\ z \\ \tau \end{pmatrix} + \begin{pmatrix} t_1 \\ t_2 \\ t_3 \\ \tau_0 \end{pmatrix}$$

R transforms **q** either to **q** or -**q**

$$\mathbf{R} \cdot \mathbf{q} = R_I \mathbf{q} + \mathbf{H_R}$$

$\mathbf{H_R} \neq \mathbf{0}$ only if a commensurate component is present, e.g.

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \begin{pmatrix} 1/2 \\ 0 \\ \delta \end{pmatrix} = \begin{pmatrix} 1/2 \\ 0 \\ \bar{\delta} \end{pmatrix} + \begin{pmatrix} \bar{1} \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} \bar{1/2} \\ 0 \\ \bar{\delta} \end{pmatrix}$$

$$\mathbf{M}'(R_I\tau + \tau_0 + \mathbf{H_R} \cdot \mathbf{r}') = \theta \det(\mathbf{R}) \mathbf{R} \cdot \mathbf{M}(\tau)$$

phase shift

same as before

Perez-Mato et al., *J. Phys.: Condens. Matter* **24** 163201 (2012)

Demonstration

Magnetic superspace groups

Example: $TbMnO_3$, *Pbnm* (#62), **q** = (0 0.27 0) using ISODISTORT (iso.byu.edu)

Kenzelmann et al., *Phys. Rev. Lett.* **95** 087206 (2005) Campbell et al., *J. Appl. Cryst.* **39** 608 (2006)

ISODISTORT: order parameter direction

Space Group: 62 Pbnm D2h-16, Lattice parameters: a= 5.29700, b= 5.83100, c= 7.40300, alpha= 90.00000, beta= 90.00000, gamma= 90.00000
Default space-group preferences: monoclinic axes a(b)c, monoclinic cell choice 1, orthorhombic axes abc, origin choice 2, hexagonal axes, SSG standard setting
Space-group preferences for parent: orthorhombic axes cab
TB 4c (x,y,1/4), x=-0.02800, y= 0.07200, MN 4b (1/2,0,0), O1 4c (x,y,1/4), x= 0.09700, y= 0.46000, O2 8d (x,y,z), x=-0.29600, y= 0.33700, z= 0.05600
Include magnetic Mn distortions
k point: SM, k8 (0,a,0), a=0.27000 (1 incommensurate modulation/1 arm)
IR: mSM3, mk8t1
k point: SM, k8 (0,a,0), a=0.27000 (1 incommensurate modulation/1 arm)
IR: mSM2, mk8t4

Finish selecting the distortion mode by choosing an order parameter direction

- P-P (a,0|0,b) 14.1.2.1.m76.2 P2_1/b.1'(a,b,0)00s, basis={(0,0,1,0),(0,1,0,1),(-1,0,0,0),(0,0,0,1)}, origin=(0,0,0,0), s=1, i=2, k-active= (0,0.27000,0)
- **P-P (a,0|b,0) 33.1.9.5.m145.2 P2_1cn.1'(0,0,g)000s, basis={(0,0,-1,0),(1,0,0,0),(0,-1,0,1),(0,0,0,1)}, origin=(0,0,0,0), s=1, i=2, k-active= (0,0.27000,0)**
- C-C (a,b|c,d) 7.1.2.1.m25.2 Pb.1'(a,b,0)0s, basis={(0,0,1,0),(0,1,0,1),(-1,0,0,0),(0,0,0,1)}, origin=(1/4,0,0,0), s=1, i=4, k-active= (0,0.27000,0)

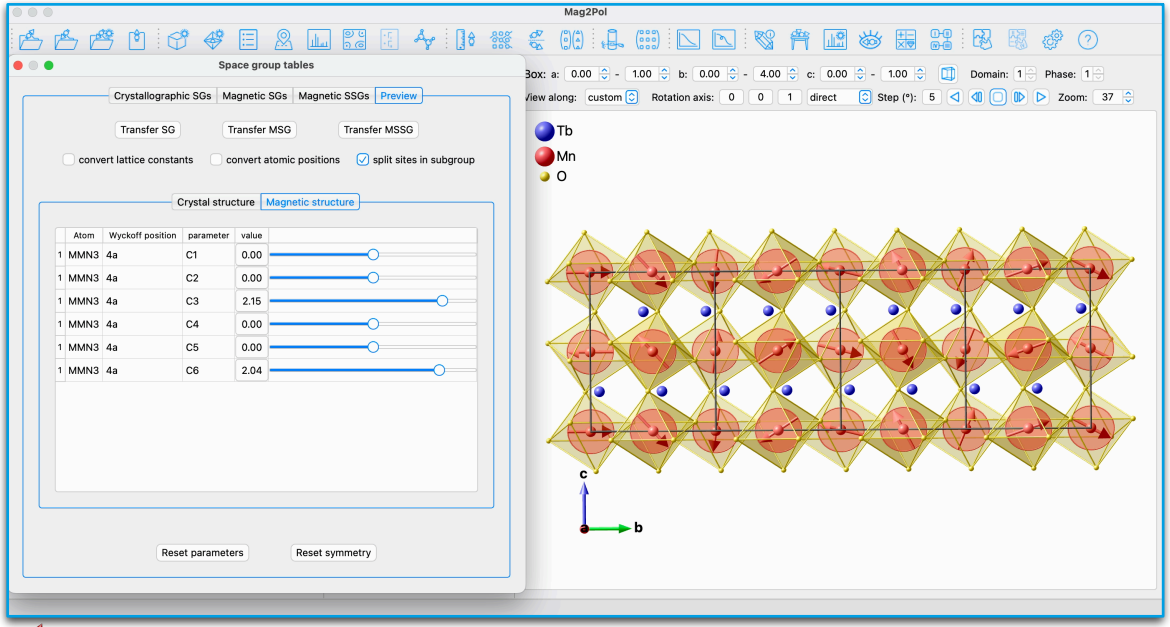
OK

Demonstration

Magnetic superspace groups

Example: $TbMnO_3$, *Pbnm* (#62), **q** = (0 0.27 0) using ISODISTORT (iso.byu.edu)

Kenzelmann et al., *Phys. Rev. Lett.* **95** 087206 (2005) Campbell et al., *J. Appl. Cryst.* **39** 608 (2006)



- support of numerical label
- MSSG transformation
- automatic splitting of sites
- test structural/magnetic d.o.f.

Conclusions

Very objective

- Mag2Pol is an easy-to-use software to prepare, perform and interpret X-ray/neutron diffraction experiments
- Flexibility in describing (magnetic) structures and refining them on multiple data sets
- Numerous useful tools to make your life easier
- Under constant development with strong connection to the user community

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Tutorials

Proposed outline

PART Ia - General overview of the program

- how to setup nuclear/magnetic structures, how to use the different tools

PART Ib - SNP data analysis on $LiNi_{0.8}Fe_{0.2}PO_4$

- Setting up nuclear/magnetic structures (Cartesian/spherical coordinates, irreps + MSG), magnetic domains, correction and refinement of SNP data

PART II - Magnetic structure analysis on $Co_{0.5}Ni_{0.5}V_3O_8$

- Refinement on powder data, determination of propagation vector, magnetic refinement using irreps, inclusion of single-crystal data

PART III - Magnetic structure analysis on CuO

- Refinement on single-crystal data, magnetic refinement using irreps, use of MAXMAGN/ISODISTORT with Mag2Pol to retrieve MSG/MSSG, refinement using mixed irreps

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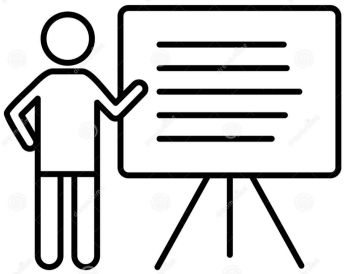

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