

Sixty Five Years of Magnetic Structures

Present and Future of Magnetic Crystallography

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Outline:

- 1. Historical introduction to neutron diffraction**
- 2. Early Magnetic Crystallography. Shubnikov Groups and Representations**
- 3. Impact of magnetic structures in condensed matter physics and chemistry**
- 4. Future of Magnetic Crystallography. Superspace groups and Representations. New computing tools**

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Historical overview:

Chadwick (1932): Discovery of the neutron (Proc Roy Soc **A136** 692)

Bloch (1936): interaction between magnetic atoms and neutrons

Schwinger (1937): QM treatment (Phys Rev **51** 544)

Alvarez and Bloch (1940): n-magnetic moment (Phys Rev **57** 111)

Halpern et al. (1937-1941): First comprehensive theory of magnetic neutron scattering (Phys Rev **51** 992; **52** 52; **55** 898; **59** 960)

Polarized neutrons milestones:

Shull et al. (1951)

Neutron Scattering and polarisation by ferromagnetic materials. Phys. Rev. **84** (1951) 912

Blume and Maleyev et al. (1963)

Polarisation effects in the magnetic elastic scattering of slow neutrons. Phys. Rev. **130** (1963) 1670

Sov. Phys. Solid State **4**, 3461

Moon et al. (1969)

Polarisation Analysis of Thermal Neutron scattering
Phys. Rev. **181** (1969) 920

History: Magnetic neutron scattering

Letters to the Editor

[The Editor does not hold himself responsible for opinions expressed by his correspondents. Neither can he undertake to return, nor to correspond with the writers of, rejected manuscripts intended for this or any other part of NATURE. No notice is taken of anonymous communications.]

Possible Existence of a Neutron

It has been shown by Bothe and others that beryllium when bombarded by α -particles of polonium emits a radiation of great penetrating power, which has an absorption coefficient in lead of about 0.3 (cm.)^{-1} . Recently Mme. Curie-Joliot and M. Joliot found, when measuring the ionisation produced by this beryllium radiation in a vessel with a thin window, that the ionisation increased when matter containing hydrogen was placed in front of the window. The effect appeared to be due to the ejection of protons with velocities up to a maximum of nearly $3 \times 10^9 \text{ cm. per sec.}$ They suggested that the transference of energy to the proton was by a process similar to the Compton effect, and estimated that the beryllium radiation had a quantum energy of $50 \times 10^6 \text{ electron volts.}$

I have made some experiments using the valve counter to examine the properties of this radiation excited in beryllium. The valve counter consists of a small ionisation chamber connected to an amplifier, and the sudden production of ions by the entry of a particle, such as a proton or α -particle, is recorded by the deflection of an oscillograph. These experiments have shown that the radiation ejects particles from hydrogen, helium, lithium, beryllium, carbon, air, and argon. The particles ejected from hydrogen behave, as regards range and ionising power, like protons with speeds up to about $3.2 \times 10^9 \text{ cm. per sec.}$ The particles from the other elements have a large ionising power, and appear to be in each case recoil atoms of the elements.

If we ascribe the ejection of the proton to a Compton recoil from a quantum of $52 \times 10^6 \text{ electron volts,}$ then the nitrogen recoil atom arising by a similar process should have an energy not greater than about 400,000 volts, should produce not more than about 10,000 ions, and have a range in air at N.T.P. of about 1.3 mm. Actually, some of the recoil atoms in nitrogen produce at least 30,000 ions. In collaboration with Dr. Feather, I have observed the recoil atoms in an expansion chamber, and their range, estimated visually, was sometimes as much as 3 mm. at N.T.P.

These results, and others I have obtained in the course of the work, are very difficult to explain on the assumption that the radiation from beryllium is a quantum radiation, if energy and momentum are to be conserved in the collision. The difficulties disappear, however, if it be assumed that the radiation consists of particles of mass 1 and charge 0, or neutrons. The capture of the α -particle by the Be^9 nucleus may be supposed to result in the formation of a C^{12} nucleus and the emission of the neutron. From the energy relations of this process the velocity of the neutron emitted in the forward direction may well be about $3 \times 10^9 \text{ cm. per sec.}$ The collisions of this neutron with the atoms through which it passes give rise to the recoil atoms, and the observed energies of the recoil atoms are in fair agreement with this view. Moreover, I have observed that the protons ejected from hydrogen by the radiation emitted in the opposite direction to that of the exciting α -particle appear to have a much smaller range than those ejected by the forward radiation.

This again receives a simple explanation on the neutron hypothesis.

If it be supposed that the radiation consists of quanta, then the capture of the α -particle by the Be^9 nucleus will form a C^{13} nucleus. The mass defect of C^{13} is known with sufficient accuracy to show that the energy of the quantum emitted in this process cannot be greater than about $14 \times 10^6 \text{ volts.}$ It is difficult to make such a quantum responsible for the effects observed.

It is to be expected that many of the effects of a neutron in passing through matter should resemble those of a quantum of high energy, and it is not easy to reach the final decision between the two hypotheses. Up to the present, all the evidence is in favour of the neutron, while the quantum hypothesis can only be upheld if the conservation of energy and momentum be relinquished at some point.

J. CHADWICK.

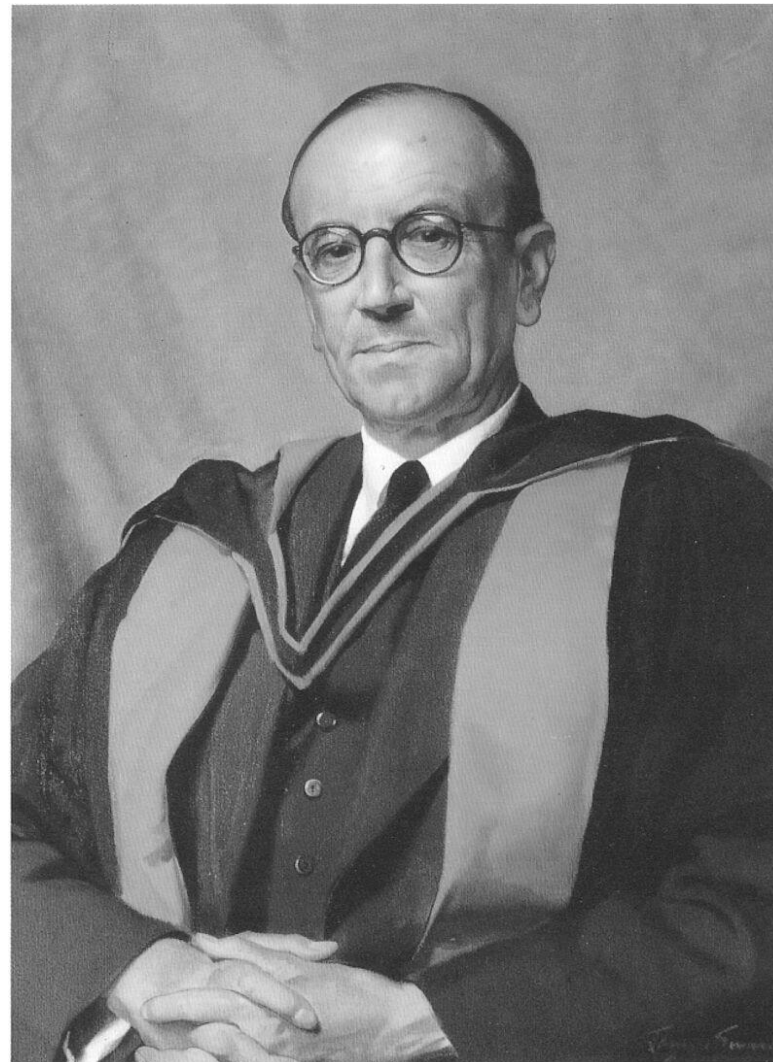
Cavendish Laboratory,
Cambridge, Feb. 17.

The Oldoway Human Skeleton

A LETTER appeared in NATURE of Oct. 24, 1931, signed by Messrs. Leakey, Hopwood, and Reek, in which, among other conclusions, it is stated that "there is no possible doubt that the human skeleton came from Bed No. 2 and not from Bed No. 4". This must be taken to mean that the skeleton is to be considered as a natural deposit in Bed No. 2, which is overlaid by the later beds Nos. 3 and 4, and that all consideration of human interment is ruled out.

If this be true, it is a most unusual occurrence. The skeleton, which is of modern type, with filed teeth, was found completely articulated down even to the phalanges, and in a position of extraordinary contraction. Complete mammalian skeletons of any age are, as field palaeontologists know, of great rarity. When they occur, their perfection can usually be explained as the result of sudden death and immediate covering by volcanic dust. Many of the more or less perfect skeletons which may be seen in museums have been rearticulated from bones found somewhat scattered as the result of death from floods, or in the neighbourhood of drying water-holes. We know of no case of a perfect articulated skeleton being found in company with such broken and scattered remains as appear to be abundant at Oldoway. Either the skeletons are all complete, as in the *Stenomylus* quarry at Sioux City, Nebraska, or are all scattered and broken in various degrees, as in ordinary bone beds. The probability, therefore, that the Oldoway skeleton represents an artificial burial is thus one that will occur to palaeontologists.

The skeleton was exhumed in 1913, and published photographs show that the excavation made for its disinterment was extensive. It is, therefore, very difficult to believe that in 1931 there can be reliable evidence left at the site as to the conditions under which it was deposited. If naturally deposited in Bed No. 2, the skeleton is of the highest possible importance, because it would be of pre-Mousterian age, and would be in the company of *Pithecanthropus* and the Pittedown, Heidelberg, and Peking men, all of whose remains are fragmentary to the last degree. Of the few other human remains for which such antiquity is claimed, the Galley Hill skeleton and the Ipswich skeleton are, or apparently were, complete. The first of these was never seen *in situ* by any trained observer, and the latter has, we believe, been withdrawn by its discoverer. The other fragments, found long ago, are entirely without satisfactory evidence as to their mode of occurrence.



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direction may well be about $3 \times 10^9 \text{ cm. per sec.}$ The collisions of this neutron with the atoms through which it passes give rise to the recoil atoms, and the observed energies of the recoil atoms are in fair agreement with this view. Moreover, I have observed that the protons ejected from hydrogen by the radiation emitted in the opposite direction to that of the exciting α -particle appear to have a much smaller range than those ejected by the forward radiation.

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On the Theory of Neutron Scattering by Magnetic Substances

In a note submitted for publication to the *Physical Review* we have suggested a new method for detecting magnetic scattering of neutrons which is based on a comparative study of paramagnetic substances with identical nuclei but varying magnetic moments. As a theoretical basis we used a letter by Bloch¹ who was the first to point out and quantitatively describe the magnetic scattering of neutrons. His results were later rederived in a quantum-theoretical treatment by Schwinger.²

Both authors have essentially treated the magnetic atom as an external field which is uninfluenced by the collision process. A complete quantum-mechanical treatment leads to the following results which for clarity, we state for different special cases.

(A) Unmagnetized paramagnetic bodies (with the magnetic ion in an S state)

The magnetic cross section is

$$\sigma = (8\pi e^4 / 3m^2 c^4) \gamma_n^2 j(j+1). \quad (1)$$

Wherein γ_n denotes the magnetic moment of the neutron in nuclear Bohr magnetons and the other symbols are self-explanatory. The result is independent of the spin-state of the incident neutron beam. It raises all values of the magnetic cross sections given in our previous note in the ratio $(j+1)/j$.

(B) Ferromagnetic bodies

Here the result depends on the energetic possibility of the spin-moment changing direction during the course

transitions to neighboring spectroscopic levels, the presence of isotopes and the existence of spin-dependent nuclear forces. The magnetic cross section on the other hand, is increased by transitions of the atoms to neighboring energy states.

In the above considerations we have refrained from including form factors which can considerably influence the results, even for thermal neutrons, but which are taken into account in our detailed calculations.

O. HALPERN

M. H. JOHNSON, JR.

New York University,
University Heights,
May 13, 1937.

¹ F. Bloch, *Phys. Rev.* **50**, 259 (1936).

² J. Schwinger, *Phys. Rev.* **51**, 544 (1937). Bloch's formula seems to be distorted by misprint; we could not verify the interpretive correction given by Schwinger.

The Ionosphere and Magnetic Storms*

It has been recognized for many years that there was some relation between magnetic storms and poor radio transmission conditions at high frequencies. It was believed that disturbances of the ionosphere produced both the magnetic storms and poor radio transmission conditions. The ideas concerning this relation were somewhat nebulous because of a lack of specific information concerning either normal or abnormal conditions of the ionosphere.

In two previous Letters to the Editor^{1,2} we have described in detail many of the specific effects which we have observed to occur in the ionosphere during and following magnetic disturbances. Our observations and conclusions have been confirmed by many other observations at the

On the Theory of Neutron Scattering by Magnetic Substances

In a note submitted for publication to the *Physical*

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MAY 15, 1939

PHYSICAL REVIEW

VOLUME 55

On the Magnetic Scattering of Neutrons

O. HALPERN AND M. H. JOHNSON

New York University, University Heights, New York, New York

(Received December 3, 1938)

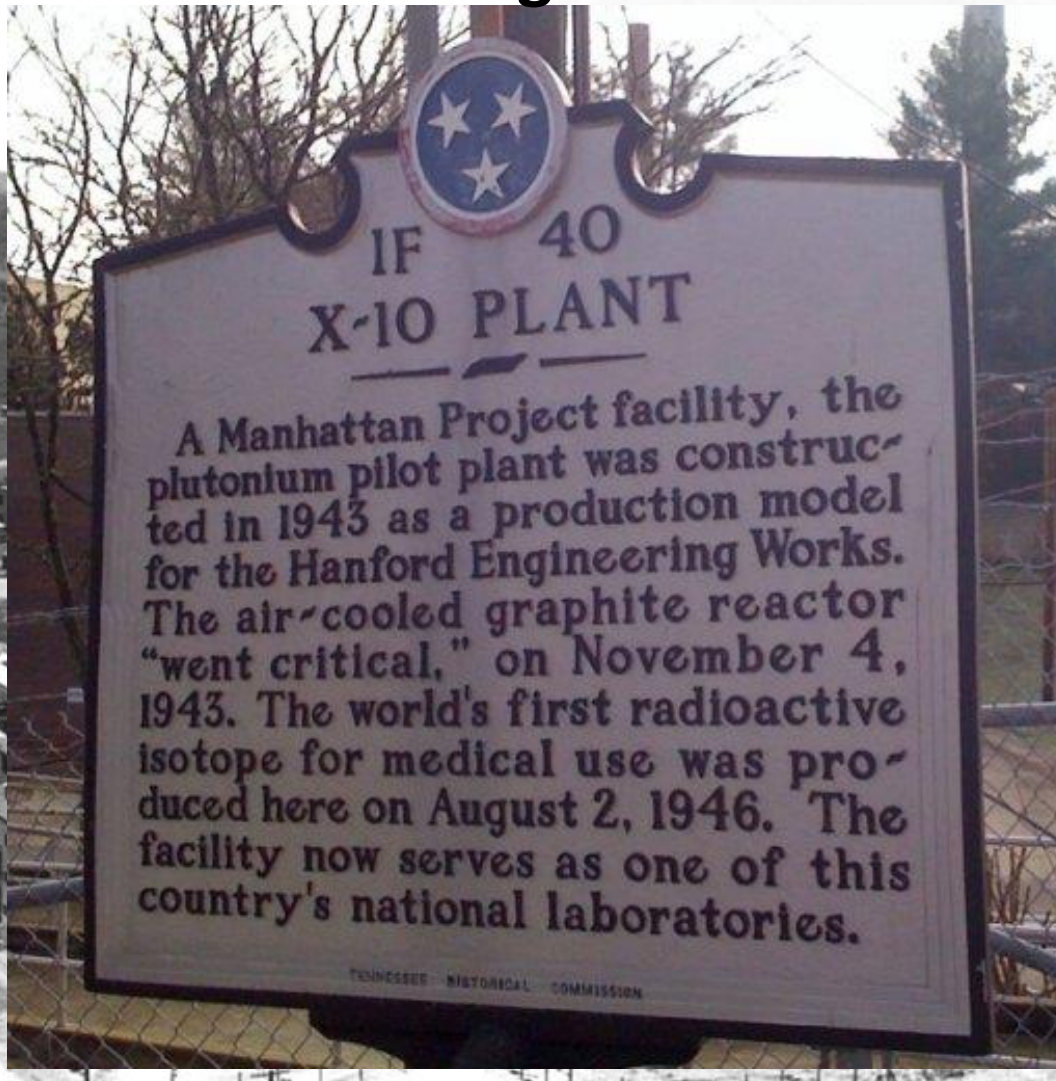
In this paper there is contained a full elaboration of two previously published short notes on the subject of magnetic scattering of neutrons together with a comprehensive treatment of certain sides of this problem which have already received some attention from other authors. After presenting the state of the problem in the introduction and discussing in detail our reasons for the choice of an interaction function between neutrons and electrons, and the nonmagnetic interaction between neutrons and nuclei, the various possible cases of coherent and incoherent scattering and depolarization phenomena are treated. Later applications to the theory of ferromagnetic scattering are kept in mind. The general expression for the cross section due to

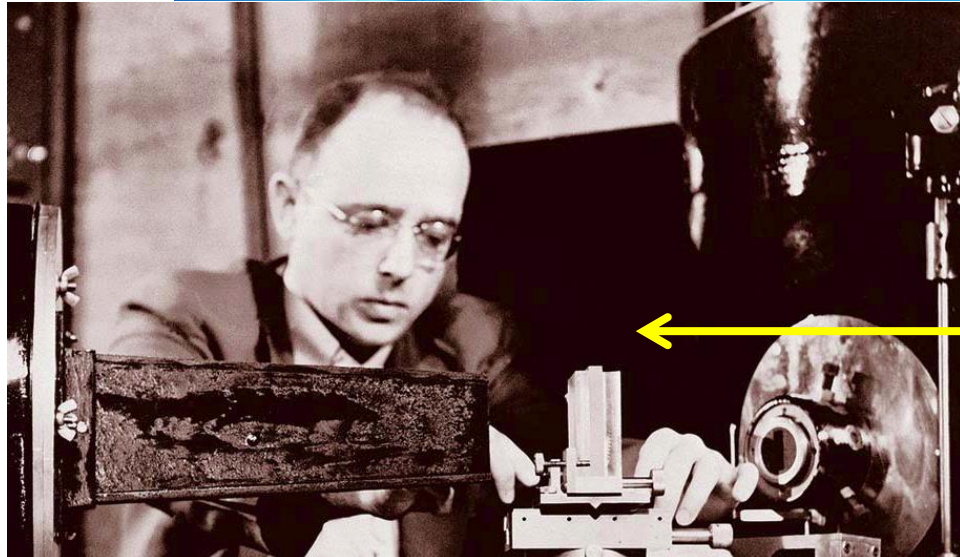
magnetic interaction is obtained and applied to various classes of phenomena (scattering by free, rigidly aligned, and coupled magnetic ions). The influence of the elastic form-factor is treated quantitatively with the aid of a simple model for the current distribution in the ion. Finally a series of performed or suggested experiments is discussed mainly from the point of view whether they will permit theoretical interpretation. Arrangements are described which will allow one to obtain a reliable value for the neutron's magnetic moment and also give insight into the magnetic constitution of the scatterer (ion or crystal) which will exceed the knowledge obtainable from macroscopic magnetic experiments.

Here the result depends on the energetic possibility of the spin moment changing direction during the course

magnetic disturbances. Our observations and conclusions have been confirmed by many other observations at the

Oak Ridge 1943

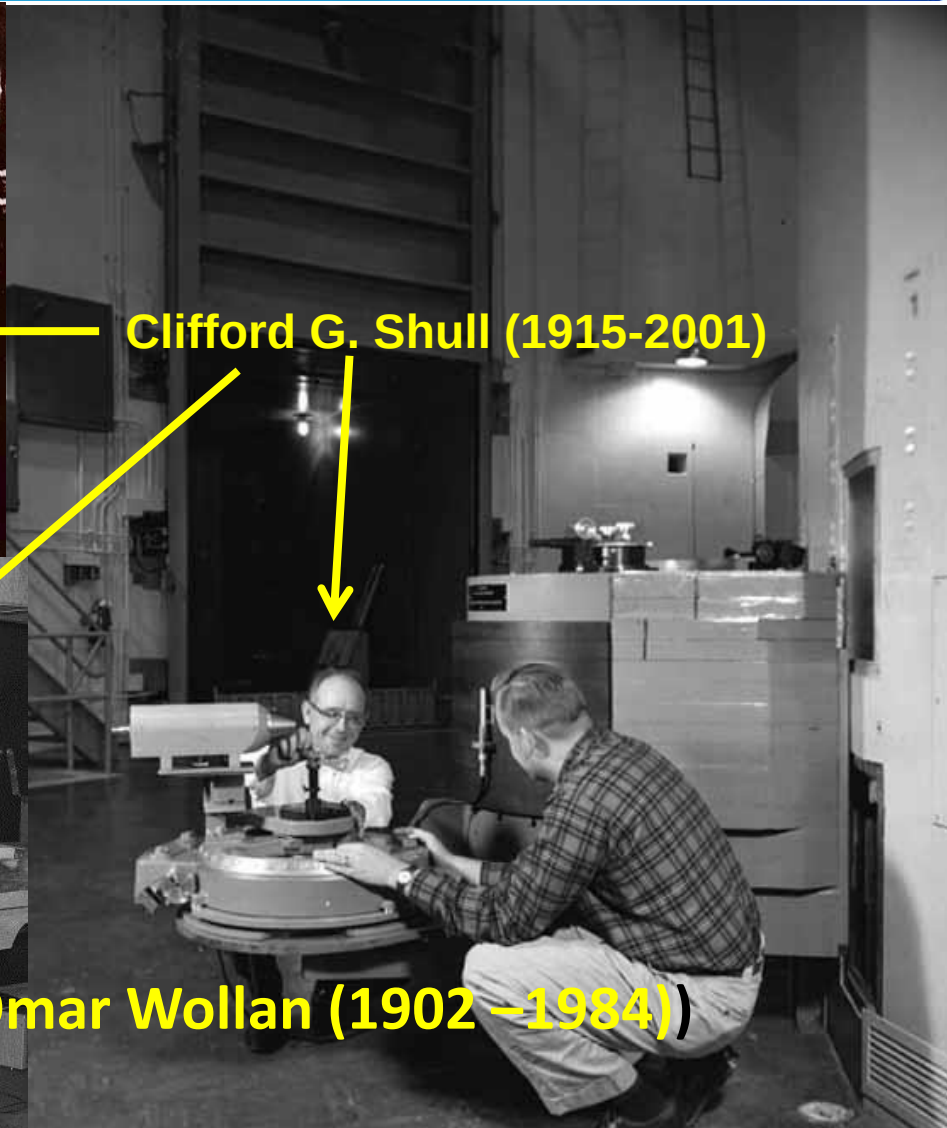




Clifford G. Shull (1915-2001)



Ernest Omar Wollan (1902 – 1984)



Clifford G. Shull: 1994 Nobel Prize winner in Physics

Physical Review **76**, 1256 (1949)

Detection of Antiferromagnetism by Neutron Diffraction*

C. G. SHULL

Oak Ridge National Laboratory, Oak Ridge, Tennessee

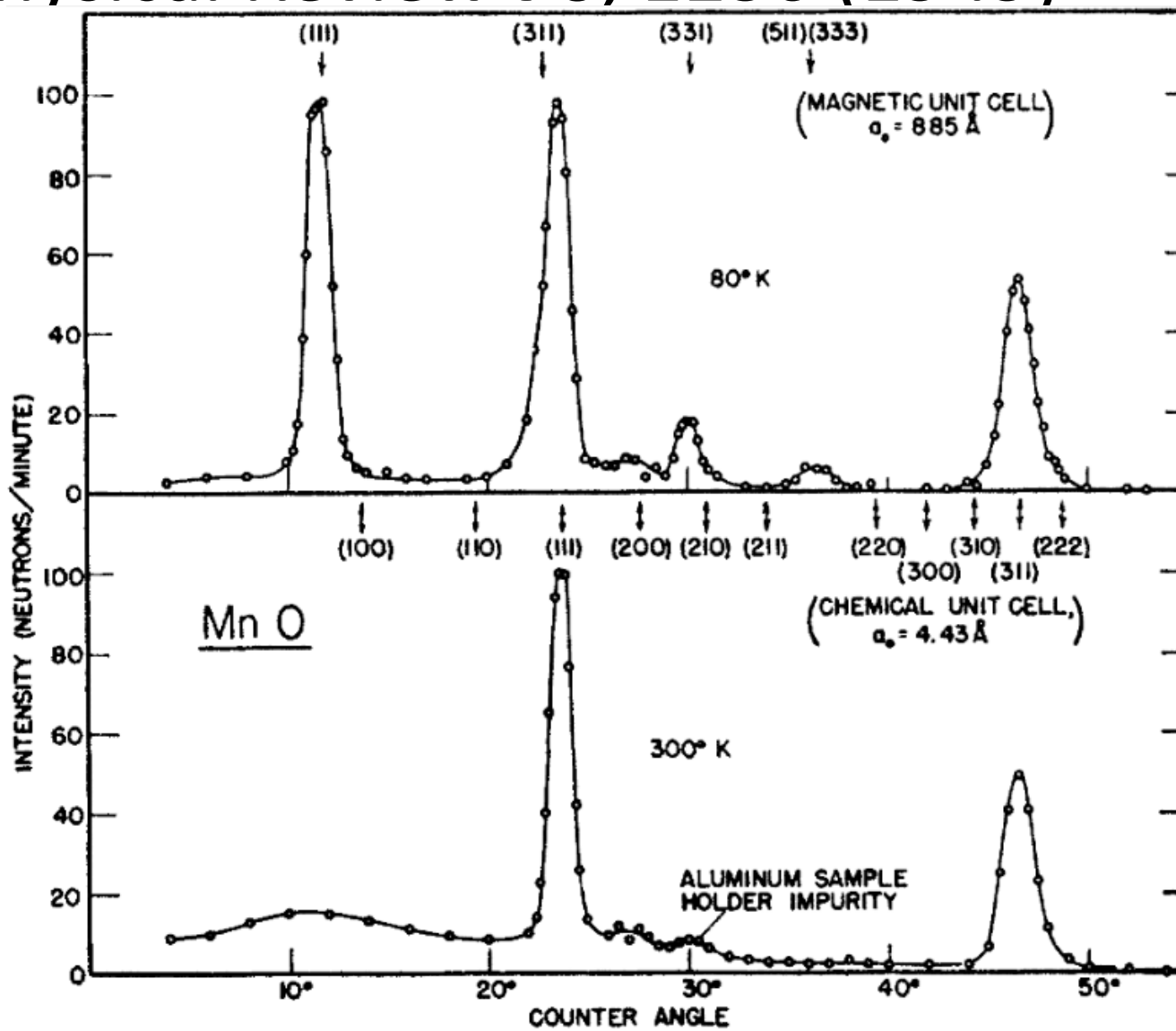
AND

J. SAMUEL SMART

Naval Ordnance Laboratory, White Oak, Silver Spring, Maryland

August 29, 1949

Physical Review **76**, 1256 (1949)



L. Neel

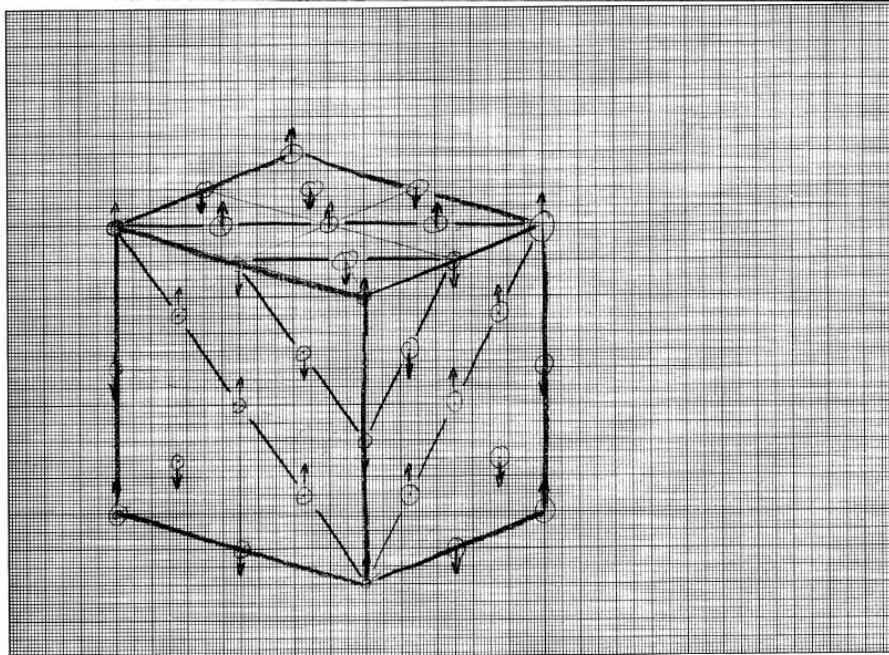
Ann. de Physique, 3 p.137 (1948)
C.R. Acad Sci Paris 228 64-6 (1949)

	MnO	MnS	FeO	FeF ₂	MnF ₂	α Fe ₂ O ₃
d (M-M)	3.12	3.68	3.03	3.36	3.30	2.91 ^{2.88} _{2.94}
d' (M-O)	2.21	2.61				

θ_m °K -610 -528

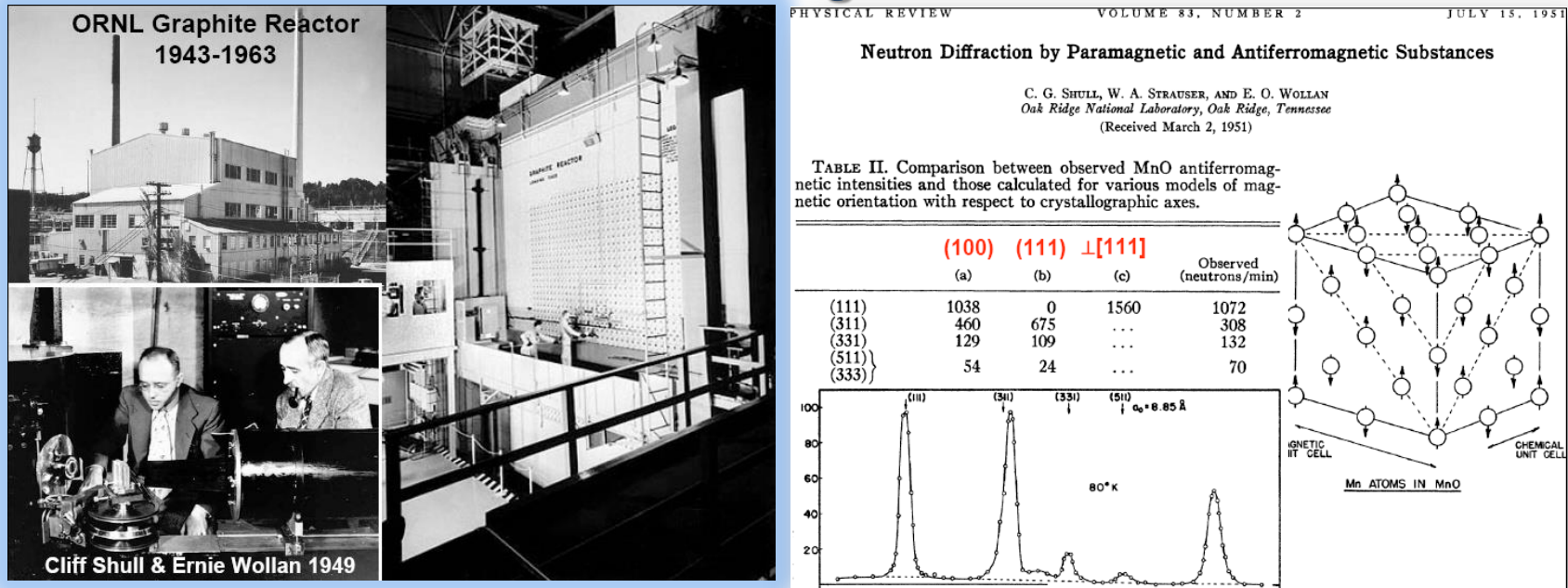
θ_p °K 122 165

c 4.4 4.3



Clifford G. Shull: 1994 Nobel Prize winner in Physics

❖ First neutron diffraction investigations of magnetic materials were done at Oak Ridge



- ✓ The first direct evidence of antiferromagnetism was produced in determining the magnetic structure of MnO
- ✓ the Néel model of ferrimagnetism was confirmed for Fe_3O_4 ,
- ✓ the first magnetic form-factor data were obtained by measuring the paramagnetic scattering by Mn compounds,
- ✓ the production of polarized neutrons by Bragg reflection from ferromagnets was demonstrated

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A crucial person in the field of magnetic structure determination was:

Felix Bertaut (1913- 2003)

Original name: Erwin Lewy,

He signed his papers as

E. F. Bertaut

***“Felix Bertaut is a mathematician who does crystallography”.
Andre Guinier***

Two (Three?) principal methods (“classifications schemes”) were developed for magnetic structure determination up to the middle of the seventies.

In terms of W. Opechowski in *Acta Cryst.* **A27**, 470 (1971):

C1: Description of magnetic structures based on conventional Shubnikov groups

W. Opechowski and R. Guccione. Magnetic Symmetry, in Magnetism, Vol. 2A, Ed. G.T. Rado and H. Suhl, Academic Press, 1965

C1': Description of magnetic structures based on non-crystallographic groups .

W. Opechowski and T. Dreyfus, *Acta Cryst* **A27**, 470 (1971).

See also: D.B. Litvin & W. Opechowski, *Spin Groups*, *Physica* **76**, 538 (1974)

W. Opechowski in *Crystallographic and Meta-crystallographic Groups*, North Holland, 1986

C2: Description of magnetic structures based on representation analysis.

See E.F. Bertaut, *Acta Cryst* **A24**, 217 (1968), Y.A. Izyumov et al., *JMMM* (1979-1980)

Two (Three?) principal methods (“classifications schemes”) were developed for magnetic structure determination up to the middle of the seventies.

In terms of W. Opechowski in *Acta Cryst.* **A27**, 470 (1971):

C1: Description of magnetic structures based on point group and spinor groups

W. Opechowski, *Acta Cryst.* **A27**, 470 (1971), Vol. 2A,

Ed. G.T. ...
I’m using C1 in a different sense as that used by Opechowski (for him C1’ includes C1 in the sense used here).

C1’: Description of magnetic structures based on point group and spinor groups.

W. Opechowski, *Acta Cryst.* **A27**, 470 (1971), Vol. 2A,

See also ... (1974)

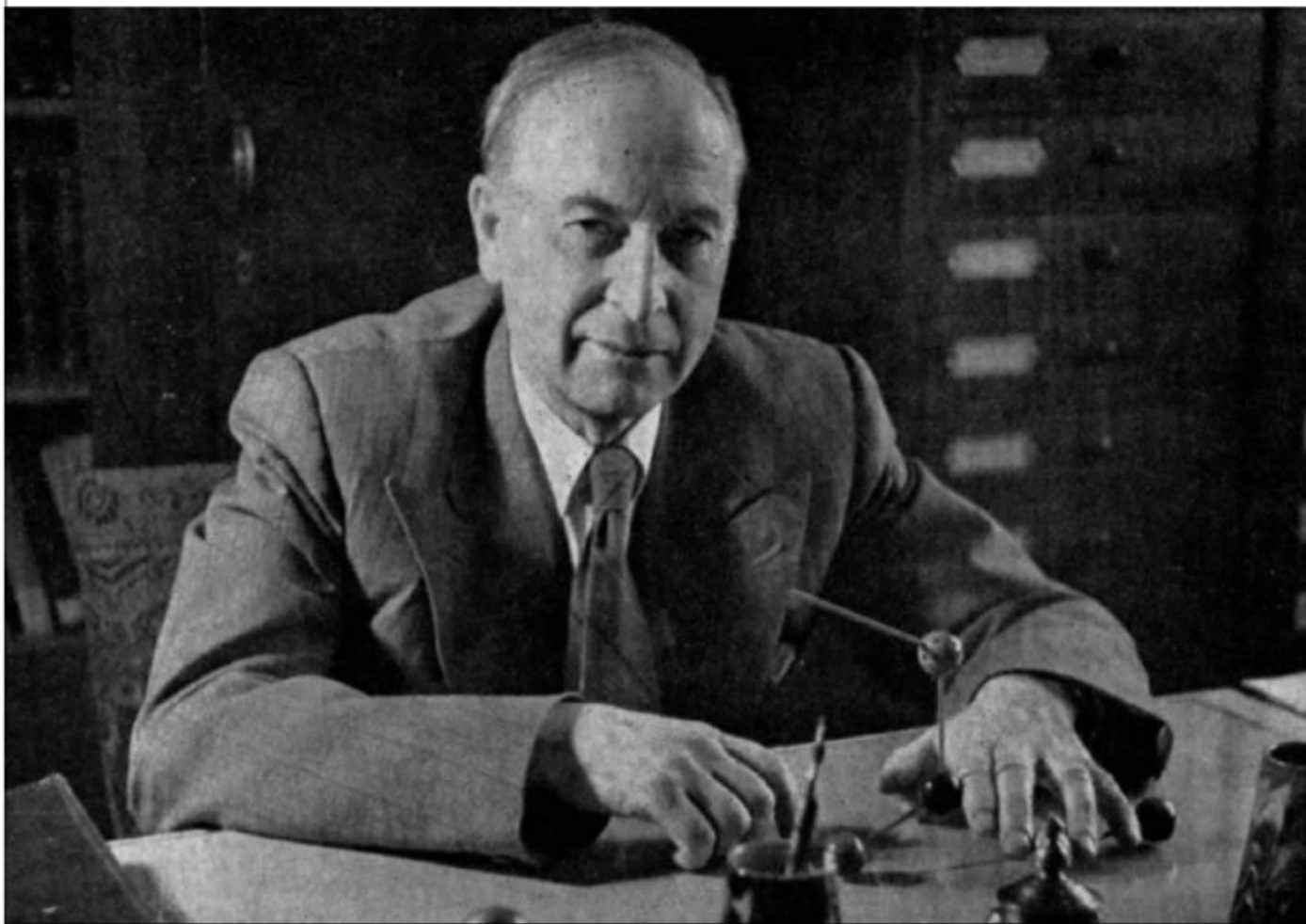
W. Opechowski, *Acta Cryst.* **A27**, 470 (1971), Vol. 2A,

Holland ...
C1 in the sense used by Opechowski is concerned with groups leaving invariant scalar functions $f(\mathbf{r})$, and C1’ is concerned with groups leaving invariant vector functions $\mathbf{B}(\mathbf{r})$

C2: Description of magnetic structures based on representation analysis.

See E.F. Bertaut, *Acta Cryst.* **A24**, 217 (1968), Y.A. Izyumov et al., *JMMM* (1979-1980)

Alexey Vasilyevich Shubnikov 1887-1970



1945: **Shubnikov** re-introduces the time reversal group $\{1, 1'\}$ first described by **Heesch** in **1929**, Z. Krist. **71**, 95.

1951: **Shubnikov** describes the bi-colour point groups

1955: **Belov, Neronova & Smirnova** provide for the first time the full list of 1651 Shubnikov space groups. Sov. Phys. Crystallogr. **1**, 487-488

1957: **Zamorzaev** derives, using group theory, the Shubnikov groups. Kristallografiya **2**, 15 (Sov. Phys. Cryst., **3**, 401)

1965: **Opechowski** and **Guccione** derive and enumerate the full list of magnetic space groups (Shubnikov groups)

1968: Describing 3-dimensional Periodic Magnetic Structures by Shubnikov Groups

Koptsik, V.A.

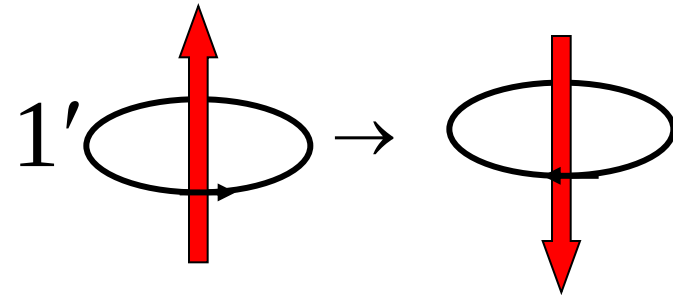
Soviet Physics Crystallography, **12** (5) , 723 (1968)

2001: **Daniel B. Litvin** provides for the first time the full description of all Shubnikov (Magnetic Space) Groups.

Acta Cryst. **A57**, 729-730

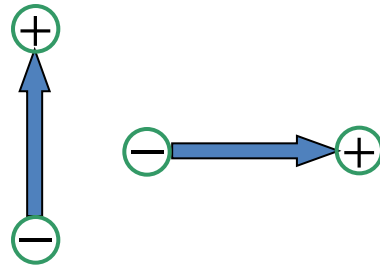
The magnetic moment (shortly called "spin") of an atom can be considered as an "axial vector". It may be associated to a "current loop". The behaviour of elementary current loops under symmetry operators can be deduced from the behaviour of the "velocity" vector that is a "polar" vector.

Time reversal = spin reversal
(change the sense of the current)

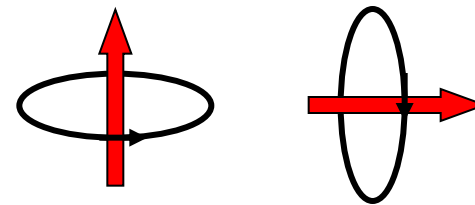


A **new operator** can be introduced and noted as **1'**, it **flips the magnetic moment**. This operator is called "spin reversal" operator or classical "time reversal" operator

Electrical dipole



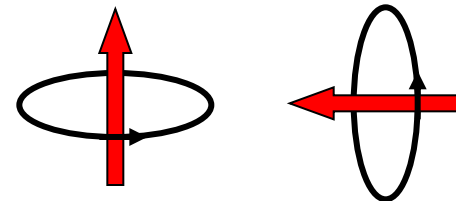
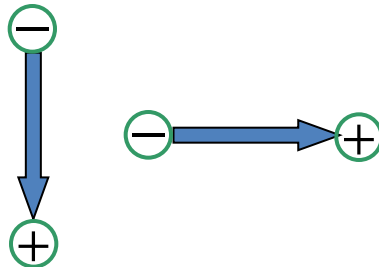
Magnetic dipole



Polar vector

Mirror plane

Axial vector



$$\mathbf{m}_j' = g\mathbf{m}_j = \det(h) \delta h \mathbf{m}_j$$

The group $R = \{1, 1'\}$ is called **the time/spin reversal group**. **Magnetic point and space groups** can be obtained as **outer direct product of point and space groups with R** . The operators of a magnetic group are called **"primed"** if they result from the combination of the crystallographic operator with the element $1'$ of R . Those combined with 1 are called **"unprimed"**.

A general operator $g = \{h | \mathbf{t}_h + \mathbf{n}\}$ acting on an atom $\mathbf{r}_j$ in the cell at the origin (zero-cell) having a magnetic moment $\mathbf{m}_j$ is transformed as follows:

$$\mathbf{r}_j' = g\mathbf{r}_j = \{h | \mathbf{t}_h + \mathbf{n}\}\mathbf{r}_j = h\mathbf{r}_j + \mathbf{t}_h + \mathbf{n} = \mathbf{r}_i + \mathbf{a}_{gj}$$

$$\mathbf{m}_j' = g\mathbf{m}_j = \det(h) \delta h \mathbf{m}_j$$

The **"signature"** is $\delta = 1$ for unprimed elements and $\delta = -1$ for primed elements

Whatever crystallographic magnetic group, M , can be obtained as a subgroup of the outer direct product of R by the crystallographic group G : $M \subset G \otimes R$.

The magnetic groups derived from the crystallographic group G can be constructed considering the index 2 subgroups H of G as constituting the "unprimed" elements and the rest of operators, $G - H$, those that are multiplied by the time reversal operator

$$M = H + (G - H) 1'$$

One obtains a total of **1651** Shubnikov groups or four different types.

T1: 230 are of the form $M_0 = G$ ("monochrome" groups)

T2: 230 of the form $P = G + G1'$ ("paramagnetic" or "grey" groups)

1191 of the form $M = H + (G - H)1'$ ("black-white", BW, groups).

T3: Among the BW group there are **674** in which the subgroup $H \subset G$ is an **equi-translation** group: **H has the same translation group as G (first kind, BW1).**

T4: The rest of black-white groups, **517**, are **equi-class** group (**second kind, BW2**). In this last family the **translation subgroup contains "anti-translations"** (pure translations associated with the spin reversal operator).

One obtains a total of **1651** Shubnikov groups or four different types.

T1: 230 are of the form $M_0=G$ ("**monochrome**" groups)

In the BW1 (Type 3) groups the subgroup of translations is the same as that of the space group of which they derive, so **the spin reversal operator is not associated with translations**: the magnetic unit cell is the same as the crystallographic cell.

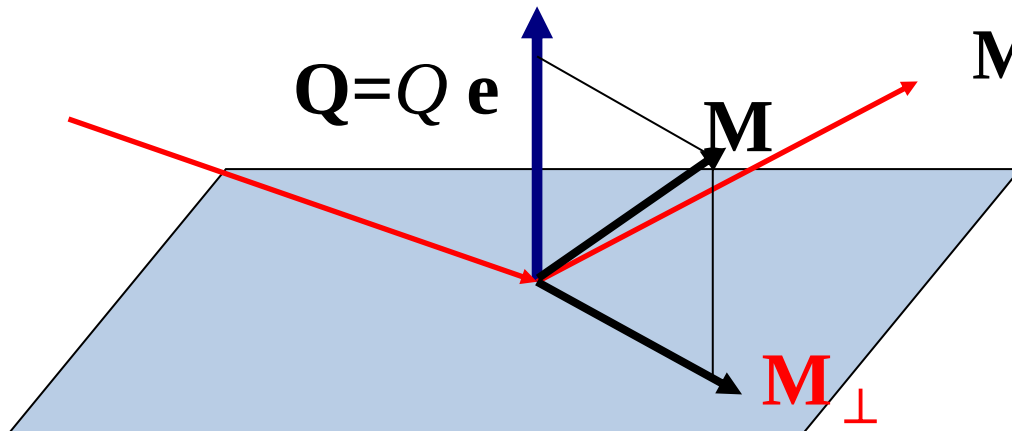
In the BW2 (Type 4) groups there are **some translations associated with spin reversal**, so that the "**magnetic unit cell**" is **bigger** than that of the crystal cell.

contains "anti-translations" (pure translations associated with the spin reversal operator).

$\mathbf{M}_{\perp}(\mathbf{Q})$ is the perpendicular component of the Fourier transform of the magnetisation in the sample to the scattering vector.

$$\mathbf{M}(\mathbf{Q}) = \int \mathbf{M}(\mathbf{r}) \exp(i\mathbf{Q} \cdot \mathbf{r}) d^3\mathbf{r}$$

Magnetic interaction vector



$$\mathbf{M}_{\perp} = \mathbf{e} \times \mathbf{M} \times \mathbf{e} = \mathbf{M} - \mathbf{e} (\mathbf{e} \cdot \mathbf{M})$$

$$I \propto \mathbf{M}_{\perp}^* \mathbf{M}_{\perp}$$

Magnetic structure factor:
$$\mathbf{M}(\mathbf{H}) = p \sum_{m=1}^{N_{mag}} \mathbf{m}_m f_m(H) \exp(2\pi i \mathbf{H} \cdot \mathbf{r}_m)$$

Neutrons only see the components of the magnetisation that are perpendicular to the scattering vector

The use of Shubnikov groups implies the use of the **magnetic unit cell** for indexing the Bragg reflections

$$\mathbf{M}_{\perp} = \mathbf{e} \times \mathbf{M} \times \mathbf{e} = \mathbf{M} - \mathbf{e} (\mathbf{e} \cdot \mathbf{M}) \quad I \propto \mathbf{M}_{\perp}^* \mathbf{M}_{\perp}$$

Magnetic structure factor:
$$\mathbf{M}(\mathbf{H}) = p \sum_{m=1}^{N_{mag}} \mathbf{m}_m f_m(H) \exp(2\pi i \mathbf{H} \cdot \mathbf{r}_m)$$

n independent magnetic sites labelled with the index j

The index s labels the representative symmetry operators of the Shubnikov group: $\mathbf{m}_{js} = \det(h_s) \delta_s h_s \mathbf{m}_j$ is the magnetic moment of the atom sited at the sublattice s of site j .

$$\mathbf{M}(\mathbf{H}) = p \sum_{j=1}^n O_j f_j(H) T_j \sum_s \det(h_s) \delta_s h_s \mathbf{m}_j \exp\{2\pi i [(\mathbf{H}\{h|\mathbf{t}\}_s \mathbf{r}_j)]\}$$

This is what we call **C1** description of magnetic structures

2001: Daniel B. Litvin provides for the first time the full description of all Shubnikov (Magnetic Space) Groups. Acta Cryst. **A57**, 729-730

<http://www.bk.psu.edu/faculty/litvin/home.html>



Magnetic Group Tables

1-, 2- and 3-Dimensional
Magnetic Subperiodic
Groups and Magnetic
Space Groups

Part 2. Tables of Magnetic Groups

Daniel B. Litvin



We are concerned here with the tables of Magnetic Groups, but many other papers from D.B. Litvin can be downloaded from its personal page at

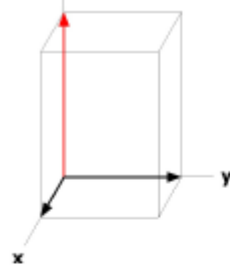
<http://www.bk.psu.edu/faculty/litvin/>

The first part is a comprehensive introduction to the tables and the second part contain each individual Magnetic Space Group item with Wyckoff positions and diagrams

Magnetic Structure Description and Determination

Group Ordering Number (BNS): 548, BNS: 62.450, OG: 59.9.486

OG: $P_{2c}m'mm$
BNS: $P_n nma$



$P_{2c}m'mn$

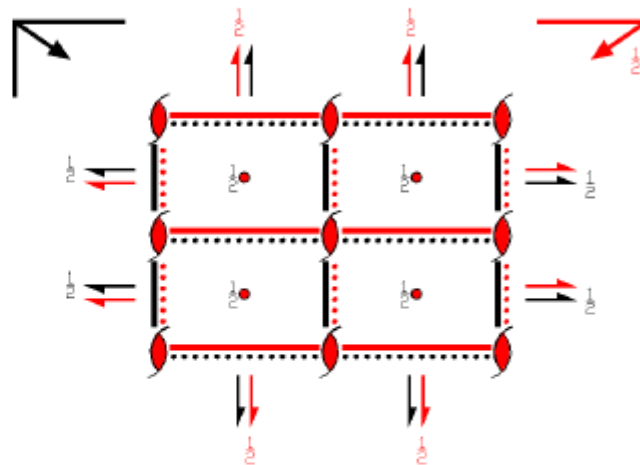
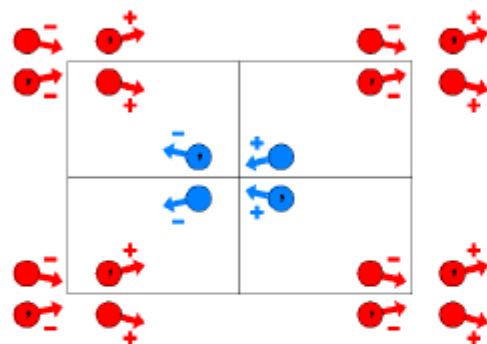
59.9.486

$mmm1'$

$P_{2c}2_1/m'2_1'/m2'/n$

Orthorhombic

OG-BNS transformation: $(1/2, 1/2, 1/2; c, -b, 2a)$



Origin at $m'm2'/n$ at $1/4, 1/4, 0$ from $\bar{1}'$

Asymmetric unit $0 \leq x \leq 1/2; 0 \leq y \leq 1/2; 0 \leq z \leq 1/2$

Symmetry Operations

For $(0,0,0) + \text{set}$

(1) 1
($1|0,0,0$)

(2) $2'$ $0,0,z$
($2_z|0,0,0'$)

(3) $2'$ $(0,1/2,0)$ $1/4,y,0$
($2_y|1/2,1/2,0'$)

(4) 2 $(1/2,0,0)$ $x,1/4,0$
($2_x|1/2,1/2,0$)

(5) $\bar{1}'$ $1/4,1/4,0$
($\bar{1}'|1/2,1/2,0'$)

(6) n $(1/2,1/2,0)$ $x,y,0$
($m_z|1/2,1/2,0$)

(7) m $x,0,z$
($m_y|0,0,0$)

(8) m' $0,y,z$
($m_x|0,0,0'$)

For $(0,0,1)' + \text{set}$

(1) $1'$ $(0,0,1)$
($1|0,0,1'$)

(2) 2 $(0,0,1)$ $0,0,z$
($2_z|0,0,1$)

(3) 2 $(0,1/2,0)$ $1/4,y,1/2$
($2_y|1/2,1/2,1$)

(4) $2'$ $(1/2,0,0)$ $x,1/4,1/2$
($2_x|1/2,1/2,1'$)

(5) $\bar{1}$ $1/4,1/4,1/2$
($\bar{1}|1/2,1/2,1$)

(6) n' $(1/2,1/2,0)$ $x,y,1/2$
($m_z|1/2,1/2,1'$)

(7) c' $(0,0,1)$ $x,0,z$
($m_y|0,0,1'$)

(8) c $(0,0,1)$ $0,y,z$
($m_x|0,0,1$)

Continued

59.9.486

P_{2c} $m'mn$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5).

Positions

Coordinates

Multiplicity,
Wyckoff letter,
Site Symmetry.

$(0,0,0) +$ $(0,0,1)'$ +

16 g 1

(1) x,y,z $[u,v,w]$	(2) $\bar{x},\bar{y},z$ $[u,v,\bar{w}]$	(3) $\bar{x}+1/2,y+1/2,\bar{z}$ $[u,\bar{v},w]$	(4) $x+1/2,\bar{y}+1/2,\bar{z}$ $[u,\bar{v},\bar{w}]$
(5) $\bar{x}+1/2,\bar{y}+1/2,\bar{z}$ $[\bar{u},\bar{v},\bar{w}]$	(6) $x+1/2,y+1/2,\bar{z}$ $[\bar{u},\bar{v},w]$	(7) $x,\bar{y},z$ $[\bar{u},v,\bar{w}]$	(8) $\bar{x},y,z$ $[\bar{u},v,w]$
8 f .m. $x,0,z$ $[0,v,0]$	$\bar{x},0,z$ $[0,v,0]$	$\bar{x}+1/2,1/2,\bar{z}$ $[0,\bar{v},0]$	$x+1/2,1/2,\bar{z}$ $[0,\bar{v},0]$
8 e m' . $0,y,z$ $[0,v,w]$	$0,\bar{y},z$ $[0,v,\bar{w}]$	$1/2,y+1/2,\bar{z}$ $[0,\bar{v},w]$	$1/2,\bar{y}+1/2,\bar{z}$ $[0,\bar{v},\bar{w}]$
8 d $\bar{1}$ $1/4,1/4,1/2$ $[u,v,w]$	$3/4,3/4,1/2$ $[u,v,\bar{w}]$	$1/4,3/4,1/2$ $[\bar{u},v,\bar{w}]$	$3/4,1/4,1/2$ $[\bar{u},v,w]$
8 c $\bar{1}'$ $1/4,1/4,0$ $[0,0,0]$	$3/4,3/4,0$ $[0,0,0]$	$1/4,3/4,0$ $[0,0,0]$	$3/4,1/4,0$ $[0,0,0]$
4 b $m'm2'$ $0,1/2,z$ $[0,v,0]$	$1/2,0,\bar{z}$ $[0,\bar{v},0]$		
4 a $m'm2'$ $0,0,z$ $[0,v,0]$	$1/2,1/2,\bar{z}$ $[0,\bar{v},0]$		

Symmetry of Special Projections

Along $[0,0,1]$ $c2mm1'$

$a^* = a$ $b^* = b$

Origin at $0,0,z$

Along $[1,0,0]$ $p2mg$

$a^* = b$ $b^* = c$

Origin at $x,1/4,0$

Along $[0,1,0]$ $p2mg1'$

$a^* = -a$ $b^* = c$

Origin at $1/4,y,0$

Only recently the magnetic space groups are available in a computer database

Magnetic Space Groups

Compiled by Harold T. Stokes and Branton J. Campbell
Brigham Young University, Provo, Utah, USA
June 2010

These data are based on data from:

Daniel Litvin, **Magnetic Space Group Types**,
Acta Cryst. **A57** (2001) 729-730.

<http://www.bk.psu.edu/faculty/litvin/Download.html>

Symmetry of Special Projections

Along $[0,0,1]$ $c2mm1'$
 $a^* = a$ $b^* = b$
Origin at $0,0,z$

Along $[1,0,0]$ $p2mg$
 $a^* = b$ $b^* = c$
Origin at $x,1/4,0$

Along $[0,1,0]$ $p2mg1'$
 $a^* = -a$ $b^* = c$
Origin at $1/4,y,0$

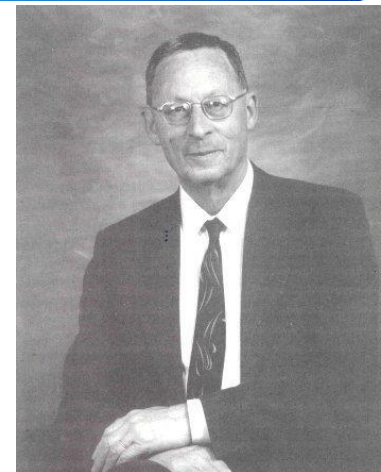
Acta Cryst. (1968). A24, 217

Representation Analysis of Magnetic Structures

BY E. F. BERTAUT

*Laboratoire d'Électrostatique et de Physique du Métal, C.N.R.S., B.P. 319 et
Laboratoire de Diffraction Neutronique, C.E.N.G., B.P. 269, Grenoble 38, France*

(Received 20 July 1967)



In the analysis of spin structures a 'natural' point of view looks for the set of symmetry operations which leave the magnetic structure invariant and has led to the development of magnetic or Shubnikov groups. A second point of view presented here simply asks for the transformation properties of a magnetic structure under the classical symmetry operations of the 230 conventional space groups and allows one to assign irreducible representations of the actual space group to all known magnetic structures. The superiority of representation theory over symmetry invariance under Shubnikov groups is already demonstrated by the fact proven here that the only invariant magnetic structures describable by magnetic groups belong to real one-dimensional representations of the 230 space groups. Representation theory on the other hand is richer because the number of representations is infinite, *i.e.* it can deal not only with magnetic structures belonging to one-dimensional real representations, but also with those belonging to one-dimensional complex and even to two-dimensional and three-dimensional representations associated with any $\mathbf{k}$ vector in or on the first Brillouin zone.

We generate from the transformation matrices of the spins a representation Γ of the space group which is reducible. We find the basis vectors of the irreducible representations contained in Γ .

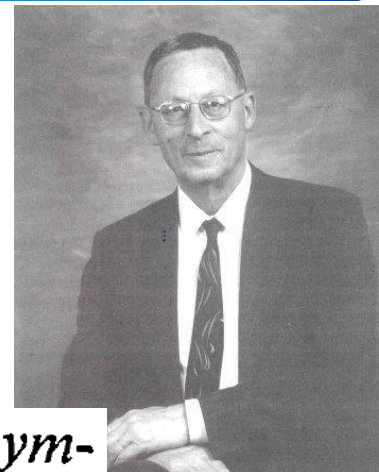
The basis vectors are linear combinations of the spins and describe the structure. The method is first applied to the $\mathbf{k}=0$ case where magnetic and chemical cells are identical and then extended to the case where magnetic and chemical cells are different ($\mathbf{k}\neq 0$) with special emphasis on $\mathbf{k}$ vectors lying on the surface of the first Brillouin zone in non-symmorphic space groups. As a specific example we consider several methods of finding the two-dimensional irreducible representations and its basis vectors associated with $\mathbf{k}=\frac{1}{2}\mathbf{b}_2=[0\frac{1}{2}0]$ in space group $Pbnm$ (D_{2h}^{16}).

Acta Cryst. (1968). A24, 217

Representation Analysis of Magnetic Structures

BY E. F. BERTAUT

*Laboratoire d'Électrostatique et de Physique du Métal, C.N.R.S., B.P. 319 et
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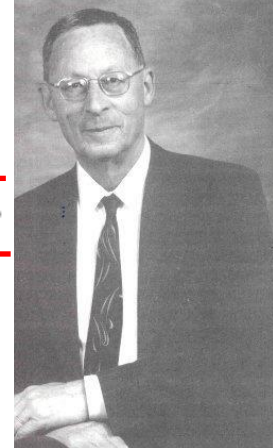
In opposition to the (widely accepted) view of symmetry invariance under the Shubnikov groups we develop in § 2 a new point of view which investigates the transformation properties of magnetic structures under the operations of the 'trivial' 230 space groups. Moreover this new point of view will prove to be more general. We show indeed that all the magnetic groups can be generated from the knowledge of the ensemble of one-dimensional real representations of the 230 space groups; in other words the 'magnetic' groups can only describe those magnetic structures which belong to one-dimensional representations, having characters $+1$ or -1 , of the classical space groups.

7. Magnetoelectricity

4

The reader may get the impression that the author is hostile to the use of magnetic groups. In fact the author is only defending representation theory. The main objection of the reader might be that in the abstract sense magnetic and space groups are isomorphous* so that a structure belonging to a representation of a space group G (even when the representation is not one-dimensional real) also belongs to a representation of the isomorphous Shubnikov group G' . This is perfectly correct, but still means that we would abandon symmetry invariance in favour of representation theory.

Can we ignore magnetic groups entirely? The answer is no, not only in microscopic, say atomic systems† (Dimmock & Wheeler, 1962) but also macroscopically when a magnetic system is coupled with other forms of energy.



Acta Cryst. (1971). A27, 470

Classifications of Magnetic Structures

BY W. OPECHOWSKI AND TOMMY DREYFUS*

Department of Physics, University of British Columbia, Vancouver, Canada

(Received 17 August 1970)

Two different classification schemes have been used for concise characterization of magnetic structures: one (called here $C1'$) making use of magnetic groups, and another, more recent (called here $C2$), in which representations of space groups play an essential part. While the mathematical principles of $C1'$ have already been formulated in all their generality, this is not so in the case of $C2$ (although many magnetic structures have been discussed from the point of view of $C2$). In this paper the principles of $C2$ are formulated in a mathematically general way, a link between $C1'$ and $C2$ is established, and a few illustrative examples of magnetic structures are discussed. It turns out that $C1'$ and $C2$ are equivalent in a precise mathematical sense, provided cyclic boundary conditions are imposed on the crystal; each magnetic structure has then its appropriate label in both classifications. If, however, one is not willing to impose such conditions, $C2$ may in some cases (as for example helical structures) meet with mathematical difficulties while $C1'$ never does. Claims made by Bertaut (*Acta Cryst.* (1968). A24, 217) that $C2$ is 'more general' than $C1'$ are thus unjustified.

Discussion of $C1$, $C1'$ and $C2$ approaches for magnetic structures

Point of view of W. Opechowski => $C1'$ is the good approach

Full discussion of **C1, C1'** and **C2** approaches for magnetic structures

Journal de Physique, Coll. C1, 32 (sup. 2-3) (1971), c1-462-460

JOURNAL DE PHYSIQUE

Colloque C 1, supplément au n° 2-3, Tome 32, Février-Mars 1971, page C 1 - 462

MAGNETIC STRUCTURE ANALYSIS AND GROUP THEORY

E. F. BERTAUT

C. N. R. S. and C. E. N.-G., rue des Martyrs, Grenoble

Résumé. — L'analyse de structures magnétiques par la théorie des groupes (analyse de représentations) est basée sur la transformation de vecteurs spins, situés dans une position cristallographique donnée, sous les opérations de symétrie d'un groupe d'espace G ou sous-groupe G_k du cristal dans lequel se trouve la structure magnétique. Le vecteur d'onde k caractérisant le groupe de translation est déduit de l'expérience de diffraction neutronique. Les équations de transformation linéaires induisent une représentation Γ de G ou de G_k . On réduit Γ en représentations irréductibles (r. i.). Les vecteurs de base, sous-tendant les r. i. décrivent des structures magnétiques possibles de sorte que l'on n'a à comparer qu'un faible nombre de modèles avec l'expérience. La symétrie de l'hamiltonien (de la représentation irréductible) est généralement plus élevée que la symétrie de Shubnikov de la structure magnétique. Quant au schéma de classification d'Opechowski, notre schéma (C2) utilise d'une manière cohérente et exclusive les *groupes d'espace*, même pour des spins sinusoïdaux et hélicoïdaux alors que dans le schéma C1' on doit ajouter des groupes *non cristallographiques* pour une description de ces cas.

Abstract. — The analysis of magnetic structures by group theory (representation analysis) is based on the transformation of spins on a given lattice site under the symmetry operations of a crystallographic space group G or a subgroup G_k of the crystal in which the magnetic structure is imbedded. The wave vector k labelling the translation group is taken from the neutron diffraction experiment. The linear transformation equations induce a representation Γ of G or G_k . Γ is reduced to irreducible representations. Basis vectors, constructed from them, describe possible magnetic structures so that only a small number of models have to be compared with experiment. The symmetry of the hamiltonian (of the irreducible representation) is generally higher than the Shubnikov symmetry of the magnetic structure. As far as Opechowski's classification scheme is concerned our scheme (C2) uses *space* groups consistently, even for sinusoidal and helical spins whereas in the scheme C1' one must add *non crystallographic* groups for a full description of the latter case.

Magnetic Structure Description and Determination

Full discussion of C1, C1' and C2 approaches for magnetic structures

Journal de Physique, Coll. C1, 32 (sup. 2-3) (1971), c1-462-460

JOURNAL DE PHYSIQUE

Colloque C 1, supplément au n° 2-3, Tome 32, Février-Mars 1971, page C 1 - 462

MAGNETIC STRUCTURE ANALYSIS AND GROUP THEORY

E. F. BERTAUT

C. N. R. S. and C. E. N.-G., rue des Martyrs, Grenoble

Introduction. — Representation analysis of a magnetic structure is not only a) labelling or classifying a structure, but consists mainly of b) the search for the structure before it is known and of c) the discussion of the interactions which might explain the final structure model. Professor Opechowski has not evaluated the merits of representation analysis for b) and c). Thus I shall answer his criticism at the end of my lecture.

Magnetic Structure Description and Determination

Discussion of C1, C1' and C2 approaches for magnetic structures

Journal de Physique, Coll. C1, 32 (sup. 2-3) (1971), c1-462-460

C1: Description of magnetic structures based on conventional Shubnikov groups

C1': Description of magnetic structures based on non-crystallographic groups.

C2: Description of magnetic structures based on representation analysis.

I have claimed the superiority of classification C 2 over that by Shubnikov groups, and *not* over the classification C 1', as defined by Professor Opechowski.

The option **C1'** developed by W. Opechowski was extended by D.B. Litvin and W. Opechowski with the concept of “spin groups” in which continuous rotation groups (Lie groups) may be used for describing helical structures {the symmetry operators are $g=(\mathcal{R} \parallel \mathbf{R} \mid \mathbf{t})$, for a helical structure $\mathbf{S}(\mathbf{r}+\mathbf{t}) = \mathcal{R} \mathbf{S}(\mathbf{r})$ }

- V.E. Naish, *Izv. Acad. Nauk, SSSR Ser. Fiz.* **27**, 1496 (1963).
- W. Opechowski and T. Dreyfus, *Classification of Magnetic Structures*, *Acta Cryst* **A27**, 470 (1971).
- D.B. Litvin, *Spin Translation Groups*, *Acta Cryst* **A29**, 651 (1973)
- D.B. Litvin & W. Opechowski, *Spin Groups*, *Physica* **76**, 538 (1974)
- W. Opechowski, *Crystallographic and Meta-crystallographic Groups*, North Holland (1986)
- R. Lifshitz and S. E. Mandel, *Magnetically ordered quasicrystals: enumeration of spin groups and calculation of magnetic selection rules*, *Acta Cryst* **A60**, 167 (2004)

The option **C1'** developed by W. Opechowski was extended by D. B.

Litvin **C1'** which

continues to be used

helical structures

helical structures

No practical expression for magnetic structure factor were provided for the general case .

- V. A search in the Web of Science with topic
- W. “spin groups” or “spin translation groups” or
- St “spin rotation groups” gives only 82 items of (3)
- D which only 3 are related to magnetic (974)
- D
- W
- G structures.

- R. Lifshitz and S. E. Mandel, *Magnetically ordered quasicrystals: enumeration of spin groups and calculation of magnetic selection rules*, Acta Cryst **A60**, 167 (2004)



Bertaut is the principal developer of the method C2

Representation analysis of magnetic structures

E.F. Bertaut, Acta Cryst. (1968). A24, 217-231

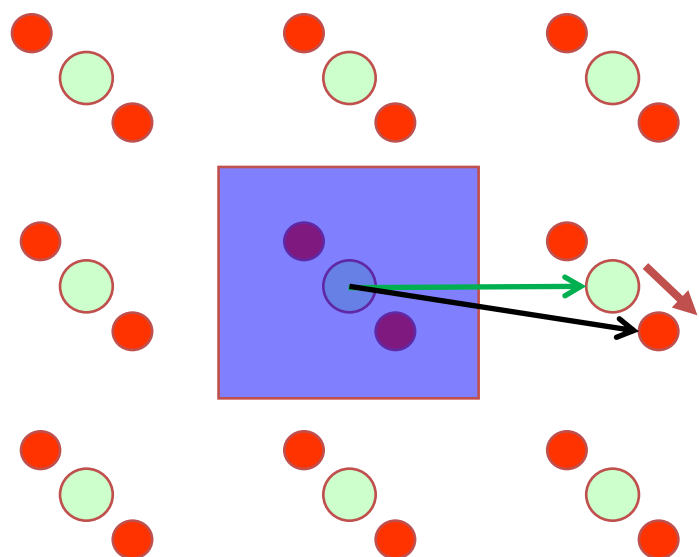


Yurii Alexandrovich Izyumov (1933-2010)

He published a series of 5 articles in **Journal of Magnetism and Magnetic Materials** on representation analysis and magnetic structure description and determination, **giving explicit and general formulae for deducing the basis functions of irreps.**

Symmetry Analysis in Neutron Diffraction Studies of Magnetic Structures, JMMM 1979-1980

Portion of reciprocal space



- Magnetic reflections
- Nuclear reflections

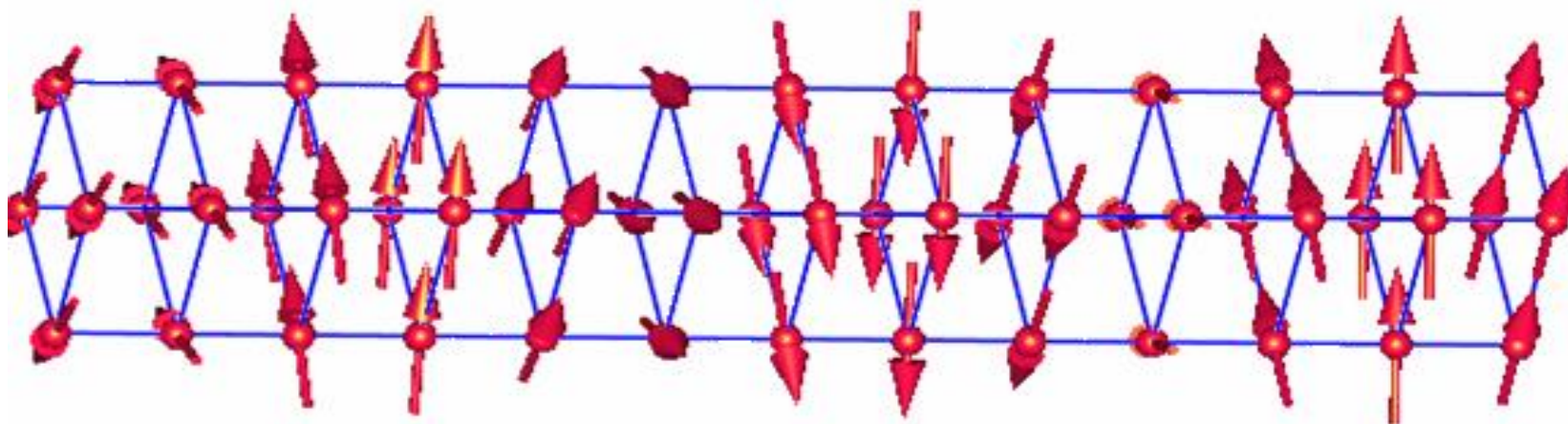
$$\mathbf{h} = \mathbf{H} + \mathbf{k}$$

Magnetic reflections: indexed by a set of propagation vectors $\{\mathbf{k}\}$

$\mathbf{h}$ is the scattering vector indexing a magnetic reflection
 $\mathbf{H}$ is a reciprocal vector of the crystallographic structure
 $\mathbf{k}$ is one of the propagation vectors of the magnetic structure
 ($\mathbf{k}$ is reduced to the Brillouin zone)

A magnetic structure is fully described by:

- i) Wave-vector(s) or propagation vector(s) $\{\mathbf{k}\}$.
- ii) Fourier components $S_{\mathbf{k}j}$ for each magnetic atom j and wave-vector $\mathbf{k}$, $S_{\mathbf{k}j}$ is a complex vector (6 components) !!!



$$\mathbf{m}_{ljs} = \sum_{\{\mathbf{k}\}} \mathbf{S}_{\mathbf{k}js} \exp\{-2\pi i \mathbf{k} \mathbf{R}_l\}$$

l : index of a direct lattice point (origin of an arbitrary unit cell)

j : index for a Wyckoff site (orbit)

s : index of a sublattice of the j site

Necessary condition for real moments $\mathbf{m}_{ljs} \Rightarrow \mathbf{S}_{-\mathbf{k}js} = \mathbf{S}_{\mathbf{k}js}^*$

General expression of the Fourier coefficients (complex vectors) for an arbitrary site (drop of js indices) when $\mathbf{k}$ and $-\mathbf{k}$ are not equivalent:

$$\mathbf{S}_{\mathbf{k}} = \frac{1}{2} (\mathbf{R}_{\mathbf{k}} + i \mathbf{I}_{\mathbf{k}}) \exp\{-2\pi i \phi_{\mathbf{k}}\}$$

Only six parameters are independent. The writing above is convenient when relations between the vectors $\mathbf{R}$ and $\mathbf{I}$ are established (e.g. when $|\mathbf{R}|=|\mathbf{I}|$, or $\mathbf{R} \cdot \mathbf{I} = 0$)

$$\mathbf{M}(\mathbf{h}) = p \sum_{j=1}^n O_j f_j(\mathbf{h}) T_j \sum_s \mathbf{S}_{\mathbf{k}js} \exp\{2\pi i[(\mathbf{H} + \mathbf{k})\{S|\mathbf{t}\}_s \mathbf{r}_j]\}$$

j : index running for all magnetic atom sites in the magnetic asymmetric unit ($j=1, \dots, n$)

s : index running for all atoms of the orbit corresponding to the magnetic site j ($s=1, \dots, p_j$). Total number of atoms: $N = \sum p_j$

$\{S|\mathbf{t}\}_s$ Symmetry operators of the propagation vector group or a subgroup

If no symmetry constraints are applied to $\mathbf{S}_{\mathbf{k}}$, the maximum number of parameters for a general incommensurate structure is $6N$ (In practice $6N-1$, because a global phase factor is irrelevant) ... we may call this method: C0

Two $\mathbf{k}$ -vectors, $\mathbf{k}$ and $\mathbf{k}'$ are equivalent if their difference is a reciprocal lattice vector: $\mathbf{k} - \mathbf{k}' = \mathbf{H}$

The set of non-equivalent $\mathbf{k}$ vectors obtained by applying the rotational part of the elements $g \in \mathbf{G}$ constitute the so called “**star of $\mathbf{k}$** ”

$$\{\mathbf{k}\} = \{\mathbf{k}_1, h_1 \mathbf{k}_1, h_2 \mathbf{k}_1, h_3 \mathbf{k}_1, \dots\} = \{\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_{l_k}\}$$

The $\mathbf{k}_i$ vectors are called the **arms of the star**. The number l_k is less or equal to the order of the point group $n(\mathbf{G}_0)$

The set of elements $g \in \mathbf{G}$ leaving the $\mathbf{k}$ vector invariant, or equal to an equivalent vector, form the group $\mathbf{G}_\mathbf{k}$. Called the **group of the wave vector** (or **propagation vector group**) or the “**little group**”. It is always a subgroup of $\mathbf{G}$. The whole space/point group (little co-group) can be decomposed in cosets of the propagation vector group:

$$\mathbf{G} = \mathbf{G}_\mathbf{k} + g_2 \mathbf{G}_\mathbf{k} + \dots = \sum_{L=1}^{l_k} g_L \mathbf{G}_\mathbf{k} \quad \mathbf{k}_L = g_L \mathbf{k}$$

We need to know the Irreps of $\mathbf{G}_k$ Γ^{kv} only for the coset representatives (with respect to the translation group) of $\mathbf{G}_k$

$$\mathbf{G}_k = 1\mathbf{T} + g_2\mathbf{T} + g_3\mathbf{T} + \dots + g_n\mathbf{T}$$

For a general element of $\mathbf{G}_k$ we have:

$$\Gamma^{kv}(\{h | \mathbf{t}_h + \mathbf{t}\}) = e^{2\pi i \mathbf{k} \cdot \mathbf{t}} \Gamma^{kv}(\{h | \mathbf{t}_h\})$$

The matrices Γ^{kv} can be easily calculated from the projective (or *loaded*) representations that are tabulated in the Kovalev book

$$\Gamma^{kv}(g) = \Gamma^{kv}(\{h | \mathbf{t}_h\}) = \Gamma_{proj}^v(h) e^{2\pi i \mathbf{k} \cdot \mathbf{t}_h}$$

The **full representations** of the space group can be obtained from the small representations by using the **induction formula**

A **reducible representation** of the propagation vector group can be constructed by selecting the atoms of a Wyckoff position and applying the symmetry operators to both positions and axial vectors. This gives rise to the so called **Magnetic Representation** of dimension: $3n_a$ (being n_a the number of atoms in the primitive cell)

This representation can be decomposed in Irreps and the number of times a particular Irreps, Γ^ν , is included can be easily calculated

$$\Gamma_{Mag} = \Gamma_{Perm} \otimes \Gamma_{Axial} = \sum_{\oplus \nu} n_\nu \Gamma^\nu$$

The basis functions, for each Irrep and each sublattice of a Wyckoff site, can be calculated by using the **projection operator formula**. The basis functions are **constant vectors** of the form (1,0,0), (0.5, 1,0) ... with components **referred to the crystallographic unitary frame**: {a/a, b/b, c/c} attached to each sublattice.

The explicit expression for the magnetic representation for the propagation vector $\mathbf{k}$, the Wyckoff position j , with sublattices indexed by (s, q) , shows that it may be considered as the direct product of the permutation representation, of dimension $p_j \times p_j$ and explicit matrices:

$$\Gamma_{Perm} \rightarrow P_{qs}^{\mathbf{k}j}(g) = e^{2\pi i \mathbf{k} \mathbf{a}_{gs}^j} \delta_{q,gs}^j \quad \text{Permutation representation}$$

by the axial (or in general “vector”) representation, of dimension 3, constituted by the rotational part of the $\mathbf{G}_{\mathbf{k}}$ operators multiplied by -1 when the operator $g = \{h | \mathbf{t}_h\}$ corresponds to an improper rotation.

$$\Gamma_{Axial} \rightarrow V_{\beta\alpha}(g) = \det(h) h_{\beta\alpha} \quad \text{Axial representation}$$

Magnetic representation

$$\Gamma_{Mag} \rightarrow \Gamma_{\beta q, \alpha s}^{\mathbf{k}j}(g) = e^{2\pi i \mathbf{k} \mathbf{a}_{gs}^j} \det(h) h_{\beta\alpha} \delta_{q,gs}^j$$



It is convenient to use, instead of the basis vectors for the whole set of magnetic atoms in the primitive cell, the so called *atomic components* of the basis vectors, which are normal 3D constant vectors attached to individual atoms:

$$\Psi_{\lambda}^{\mathbf{k}\nu}(j) = \sum_{\oplus, s=1, \dots, p_j} \mathbf{S}_{\lambda}^{\mathbf{k}\nu}(js)$$

The explicit expression provided by Yu. A. Izyumov for the atomic components of the basis functions is:

$$\mathbf{S}_{\lambda}^{\mathbf{k}\nu}(js) \propto \sum_{g \in \mathbf{G}_{0\mathbf{k}}} \Gamma_{\lambda[\mu]}^{*\nu}(g) e^{2\pi i \mathbf{k} \cdot \mathbf{a}_{gs}^j} \det(h) \delta_{s,g[q]}^j \begin{pmatrix} h_{1\alpha} \\ h_{2\alpha} \\ h_{3\alpha} \end{pmatrix}$$

$$\text{Fourier coeff.} \rightarrow \mathbf{S}_{\mathbf{k}j\mathbf{s}} = \sum_{n\lambda} C_{n\lambda}^{\nu} \mathbf{S}_{n\lambda}^{\mathbf{k}\nu} (j\mathbf{s}) \leftarrow \text{Basis vectors}$$

The coefficients $C_{n\lambda}^{\nu}$ are the free parameters of the magnetic structure.

Called “mixing coefficients” by Izyumov

Indices:

$\mathbf{k}$: reference to the propagation vector

ν : reference to the irreducible representation Γ^{ν}

n : index running from 1 up to $n_{\nu} \Rightarrow \Gamma_{Mag} = \sum_{\oplus \nu} n_{\nu} \Gamma^{\nu}$

λ : index running from 1 up to $\dim(\Gamma^{\nu})$

The fundamental hypothesis of the Symmetry Analysis of magnetic structures is that the Fourier coefficients of a magnetic structure are linear combinations of the basis functions of the irreducible representation of the propagation vector group $\mathbf{G}_{\mathbf{k}}$, the “extended little group” $\mathbf{G}_{\mathbf{k},-\mathbf{k}}$ or the full space group $\mathbf{G}$.

$$\mathbf{S}_{\mathbf{k}js} = \sum_{n\lambda} C_{n\lambda}^{\nu} \mathbf{S}_{n\lambda}^{\mathbf{k}\nu} (js) \quad \text{C2-a}$$


$$\mathbf{M}(\mathbf{h}) = p \sum_{j=1}^n O_j f_j(\mathbf{h}) T_j \sum_{n\lambda} C_{n\lambda}^{\nu} \sum_s \mathbf{S}_{n\lambda}^{\mathbf{k}\nu} (js) \exp\{2\pi i \mathbf{h}_s \mathbf{r}_j\}$$

Alternatively, a more close to traditional crystallographic approaches can be considered in some cases. The Fourier component $\mathbf{k}$ of the magnetic moment of atom j_1 , that transforms to the atom j_s when the symmetry operator $g_s = \{h|t\}_s$ of $G_{\mathbf{k}}$ is applied ($\mathbf{r}_s^j = g_s \mathbf{r}_{j_1}^j = h \mathbf{r}_{j_1}^j + \mathbf{t}_s$), is transformed as:

$$\mathbf{S}_{\mathbf{k}j_s} = M_{j_s} \mathbf{S}_{\mathbf{k}j_1} \exp\{-2\pi i \phi_{\mathbf{k}j_s}\} \quad \text{C2-b}$$

$$\mathbf{M}(\mathbf{h}) = p \sum_{j=1}^n O_j f_j(\mathbf{h}) T_j \sum_s \mathbf{S}_{\mathbf{k}j_s} \exp\{2\pi i [(\mathbf{H} + \mathbf{k})] \{h|\mathbf{t}\}_s \mathbf{r}_j - \Phi_{\mathbf{k}j}\}$$

The matrices M_{j_s} and phases $\phi_{\mathbf{k}j_s}$ can be deduced from the relations between the Fourier coefficients and atomic basis functions. The matrices M_{j_s} correspond, in the case of commensurate magnetic structures, to the rotational parts of the magnetic Shubnikov group acting on magnetic moments.

The maximum number of free coefficients to describe the magnetic structure is proportional to the number m of independent basis vectors

if we consider real coefficients when $\mathbf{k} = \frac{1}{2} \mathbf{H}$

$$n_f = m \times \dim(\Gamma^\vee)$$

if we consider complex coefficients when $\mathbf{k} \in \text{IBZ}$

$$n_f = 2m \times \dim(\Gamma^\vee) - 1$$

The analysis is successful when one of the following conditions apply:

$$n_f = 2m \times \dim(\Gamma^\vee) - 1 < 6p_j \text{ (for } \mathbf{k} \text{ non equivalent to } -\mathbf{k})$$

$$n_f = m \times \dim(\Gamma^\vee) < 3p_j \text{ (for } \mathbf{k} \text{ equivalent to } -\mathbf{k})$$

Where p_j is the number of sublattices (atoms) of site j . The effective number of free parameters is lower in general as soon as one uses the relation between basis vectors of different arms of the star $\{\mathbf{k}\}$ or select special direction in representation space for $\dim(\Gamma^\vee) > 1$.

1. Historical introduction to neutron diffraction
2. Early Magnetic Crystallography. Shubnikov Groups and Representations
- 3. Impact of magnetic structures in condensed matter physics and chemistry**
4. Future of Magnetic Crystallography. Superspace groups and Representations. New computing tools

The impact of the magnetic structures as a field in physics and chemistry of condensed matter is strongly related to

- (1) the availability of computing tools for handling the neutron diffraction data and to
- (2) the appearance of relevant topics in new materials.

Search in the Web of Science, **TOPIC:** (("magnetic structures" or "magnetic structure" or "spin configuration" or "magnetic ordering" or "spin ordering") and ("neutron" or "diffraction" or "refinement" or "determination"))

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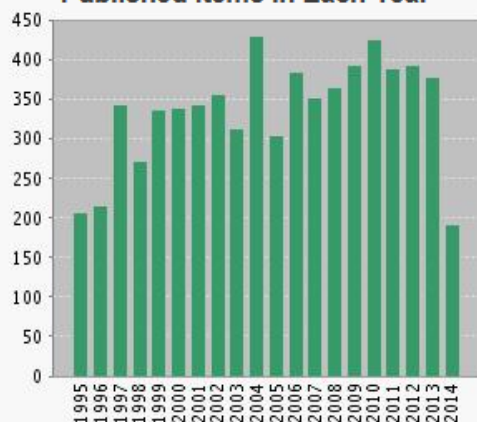
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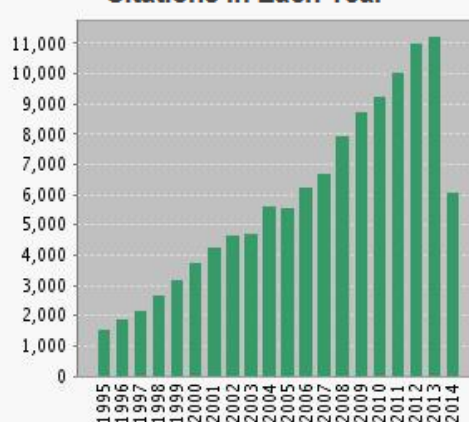
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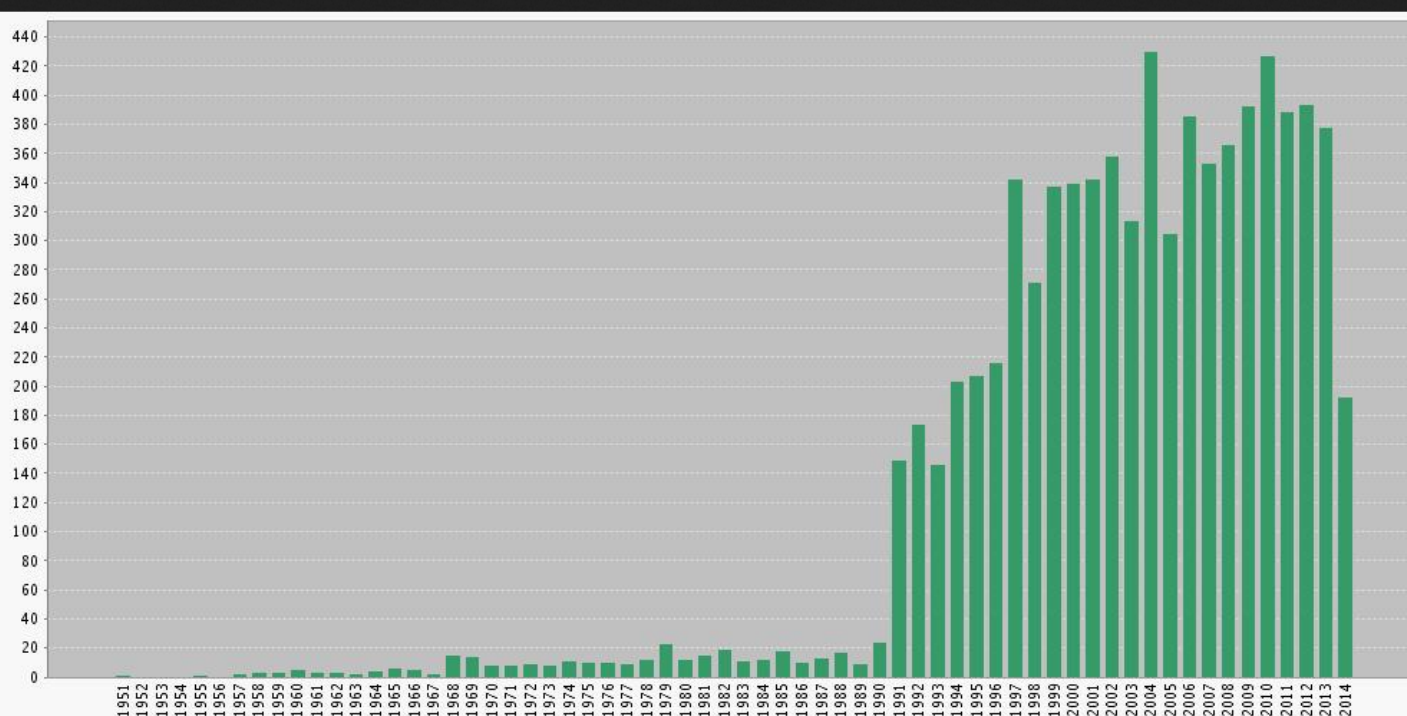
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Times Cited: 8,058

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2. **RECENT ADVANCES IN MAGNETIC-STRUCTURE DETERMINATION BY NEUTRON POWDER DIFFRACTION**

By: RODRIGUEZCARVAJAL, J

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Sponsor(s): INST LAUE LANGEVIN; EUROPEAN SYNCHROTRON RADIAT FACIL
PHYSICA B Volume: 192 Issue: 1-2 Pages: 55-69 Published: OCT 1993

Times Cited: 4,612

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By: Kimura, T; Goto, T; Shintani, H; et al.

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4. **Magnetic order close to superconductivity in the iron-based layered LaO(1-x)F(x)FeAs systems**

By: de la Cruz, Clarina; Huang, Q.; Lynn, J. W.; et al.

NATURE Volume: 453 Issue: 7197 Pages: 899-902 Published: JUN 12 2008

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5. **Physics and Applications of Bismuth Ferrite**

By: Catalan, Gustau; Scott, James F.

ADVANCED MATERIALS Volume: 21 Issue: 24 Pages: 2463-2485 Published: JUN 26 2009

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Nano particles

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- ☐ NOTE (39)

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6. **Magnetic nanoparticles** Times Cited: 767
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By: Kodama, RH
JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS Volume: 200 Issue: 1-3 Pages: 359-372 Published: OCT 1999

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7. **Charge, orbital, and magnetic ordering in La_{0.5}Ca_{0.5}MnO₃** Times Cited: 699
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By: Radaelli, PG; Cox, DE; Marezio, M; et al.
PHYSICAL REVIEW B Volume: 55 Issue: 5 Pages: 3015-3023 Published: FEB 1 1997

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8. **Magnetic inversion symmetry breaking and ferroelectricity in TbMnO₃** Times Cited: 433
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By: Kenzelmann, M; Harris, AB; Jonas, S; et al.
PHYSICAL REVIEW LETTERS Volume: 95 Issue: 8 Article Number: 087206 Published: AUG 19 2005

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9. **Direct observation of charge and orbital ordering in La_{0.5}Sr_{1.5}MnO₄** Times Cited: 426
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10. **Thermodynamic and electron diffraction signatures of charge and spin ordering in La_{1-x}CaxMnO₃** Times Cited: 412
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By: Ramirez, AP; Schiffer, P; Cheong, SW; et al.
PHYSICAL REVIEW LETTERS Volume: 76 Issue: 17 Pages: 3188-3191 Published: APR 22 1996

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(from Web of Science Core Collection)

By: Kawano, H; Kajimoto, R; Yoshizawa, H; et al.
PHYSICAL REVIEW LETTERS Volume: 78 Issue: 22 Pages: 4253-4256 Published: JUN 2 1997

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12. **Onset of antiferromagnetism in heavy-fermion metals** Times Cited: 362
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By: Schroder, A; Aeppli, G; Coldea, R; et al.

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Thin Films

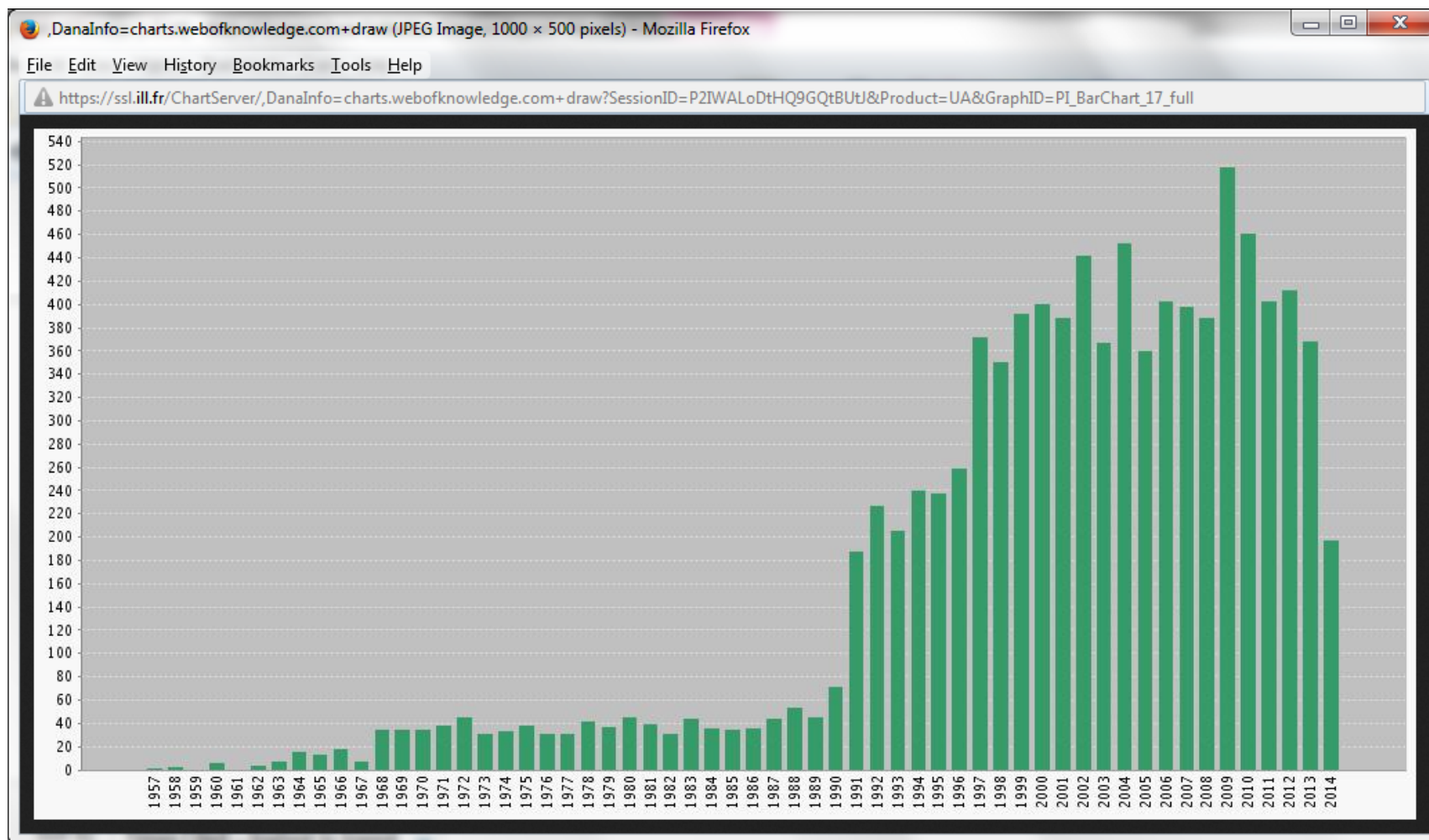
4. **ENHANCED MAGNETORESISTANCE IN LAYERED MAGNETIC-STRUCTURES WITH ANTIFERROMAGNETIC INTERLAYER EXCHANGE**
By: BINASCH, G; GRUNBERG, P; SAURENBACH, F; et al.
PHYSICAL REVIEW B Volume: 39 Issue: 7 Pages: 4828-4830 Published: MAR 1 1989

Times Cited: 1,847
(from Web of Science Core Collection)

5. **LAYERED MAGNETIC-STRUCTURES - EVIDENCE FOR ANTIFERROMAGNETIC COUPLING OF FE LAYERS ACROSS CR INTERLAYERS**
By: GRUNBERG, P; SCHREIBER, R; PANG, Y; et al.
PHYSICAL REVIEW LETTERS Volume: 57 Issue: 19 Pages: 2442-2445 Published: NOV 10 1986

Times Cited: 1,516
(from Web of Science Core Collection)

Search in the Web of Science: “Magnetic structure” or “magnetic structures” and removing non-concerned research areas.



The breakthrough: the Rietveld method



Hugo Rietveld had the idea of modelling the whole profile of the powder diffraction pattern.

Hugo M. Rietveld received the Gregori Aminoff Prize in 1995.

H.M. Rietveld distributed a least squares computer program allowing to refine crystal and magnetic structures from neutron powder diffraction patterns

A Profile Refinement Method for Nuclear and Magnetic Structures

H.M. Rietveld

Reactor Centrum Nederland, Petten (N-H.), The Netherlands

Journal of Applied Crystallography 2, 65 (1969)

The original Rietveld program was limited to commensurate magnetic structures, but his idea gave rise to a series of Rietveld programs that extended the method.

DBW, LHPM-Rietica, BGMN, BRASS, WinMProf, XND ... (no magnetism)

GSAS, RIETAN, ... (commensurate magnetic structures)

FullProf, SIMREF, JANA (incommensurate magnetic structures)

<https://www.ill.eu/sites/ccsl/html/ccsldoc.html>

Single Crystal data

The Cambridge Crystallography Subroutine Library

JC Matthewman, P Thompson and PJ Brown

J. Appl. Cryst. **15**, 167-173 (1982).

"The Cambridge Crystallography Subroutine Library (CCSL) is a set of subroutines which are used in the construction of Fortran crystallographic programs. **CCSL has been written with the needs of the nonstandard crystallographer in mind., the aim of CCSL is to allow each user to do something a little different, and to experiment with his own ideas using the subroutines in the library for the routine parts of the calculations"**



Mostly single Crystal data

Together with many “main programs” and utilities for crystallographic applications, the magnetic programs based in C^{CSL} are able to treat single crystal diffraction data (polarized and un-polarized neutrons) and also powder diffraction.

MAGLSQ : Refinement of magnetic structures (commensurate and incommensurate), treatment of flipping ratios for spin densities, etc.

CHILSQ : Refinement of local susceptibility tensors using polarized neutrons

Recent advances in magnetic structure determination by neutron powder diffraction

Physica B 192, 55 (1993)

Juan Rodríguez-Carvajal

*Laboratoire Léon Brillouin (CEA-CNRS), Centre d'Etudes de Saclay, Gif sur Yvette, France and
Institut Laue–Langevin, Grenoble, France*

In spite of intrinsic limitations, neutron powder diffraction is, and will still be in the future, the primary and most straightforward technique for magnetic structure determination. In this paper some recent improvements in the analysis of magnetic neutron powder diffraction data are discussed. After an introduction to the subject, the main formulas governing the analysis of the Bragg magnetic scattering are summarized and shortly discussed. Next, we discuss the method of profile fitting without a structural model to get precise integrated intensities and refine the propagation vector(s) of the magnetic structure. The simulated annealing approach for magnetic structure determination is briefly discussed and, finally, some features of the program FullProf concerning the magnetic structure refinement are presented and discussed. The different themes are illustrated with simple examples.

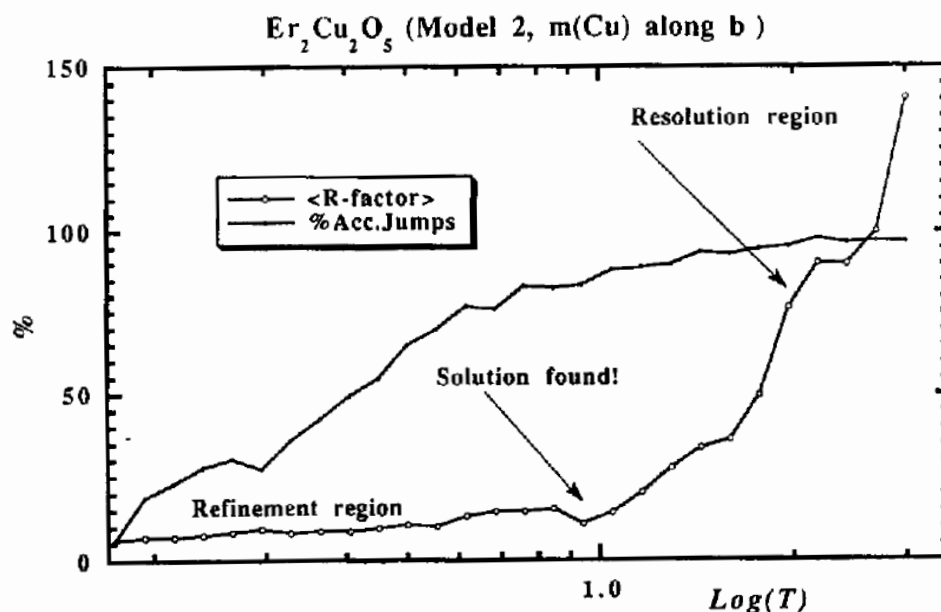
J. Rodriguez-Carvajal, Physica B 192, 55 (1993)

First description of some features of the program **FullProf**

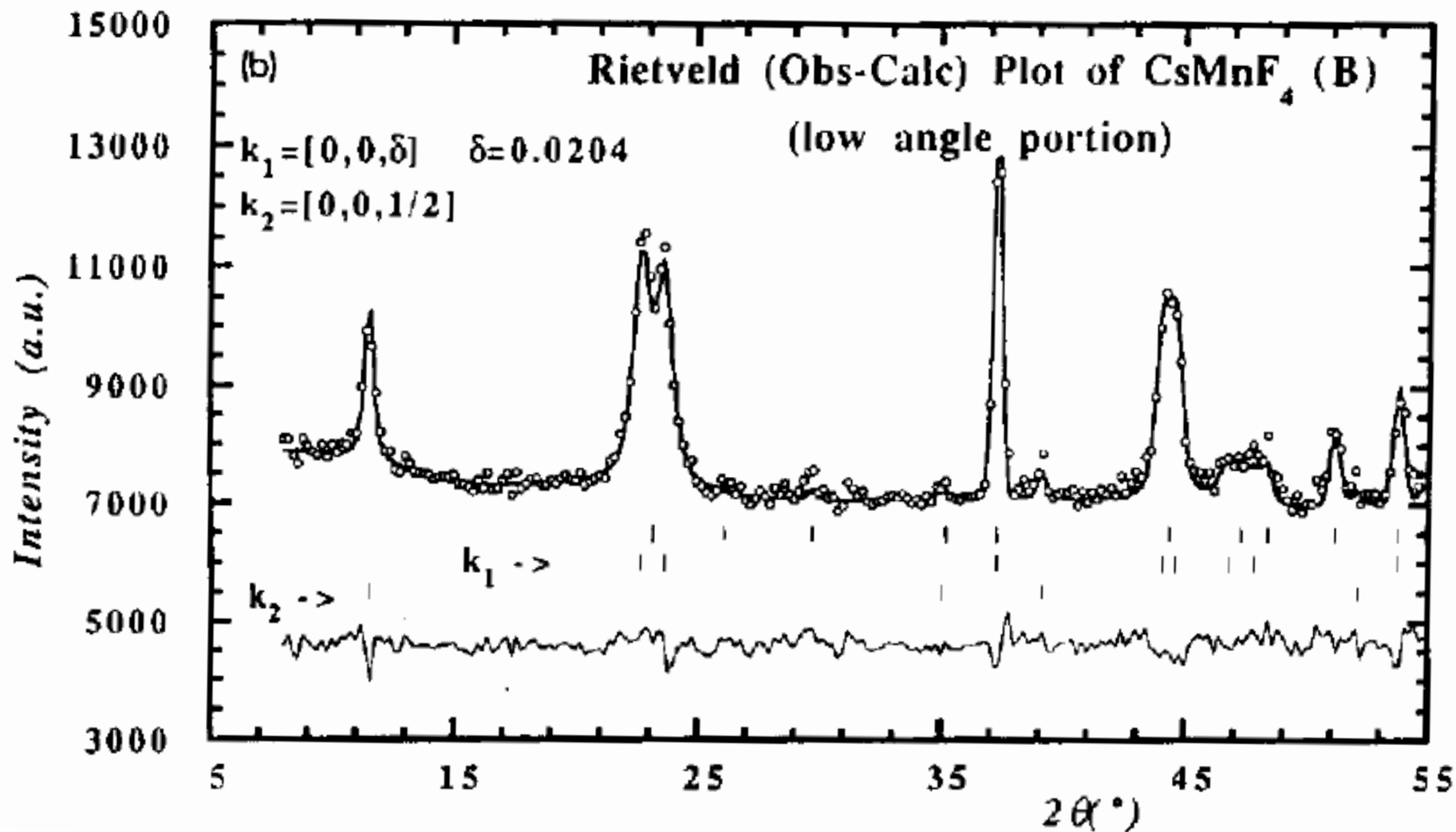
Description of the program **MagSan** for determining commensurate magnetic structures using Simulated Annealing (later included in **FullProf** for general structures)

```

begin
  Initialize (set to zero useful quantities, do preliminary
             calculations)
   $\tau = 1$ 
  do
    do
      Perturb the system:
       $\Omega_{old} \rightarrow \Omega_{new}, \Delta = E(\Omega_{new}) - E(\Omega_{old})$ 
      if  $\Delta \leq 0$  then accept, else
        if  $\exp(-\Delta/T_\tau) > \text{random}[0,1]$  then accept
      if accept then Update (replace  $\Omega_{old}$  by  $\Omega_{new}$ )
    until equilibrium is approached closely enough (Ncyc)
     $T_{\tau+1} = f(T_\tau)$  (decrease temperature, usually  $T_{\tau+1} = qT_\tau$ ,
                       $q \approx 0.9$ )
     $\tau = \tau + 1$ 
  until stop criterion is true (maximum  $\tau$ , convergence, low
    % accepted. . .)
end
  
```



J. Rodriguez-Carvajal, Physica B 192, 55 (1993)

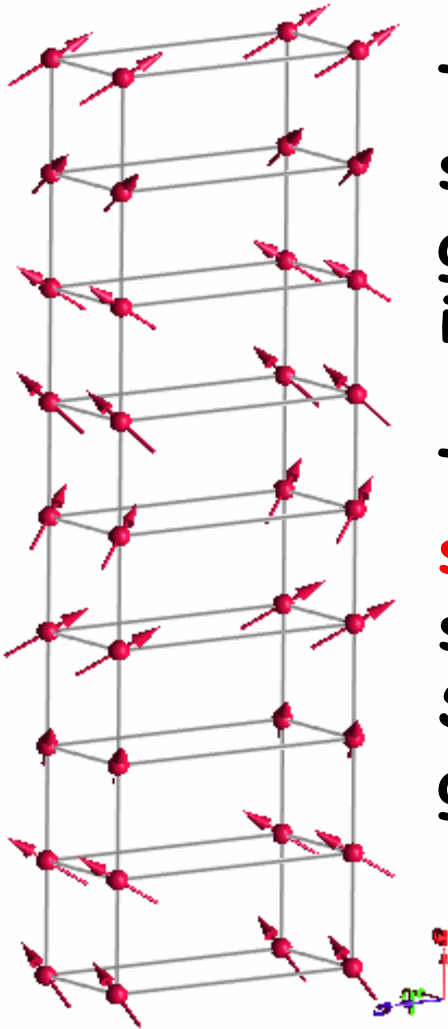


Many examples of magnetic structures have been presented in this Congress of the IUCr and none will be described here.

It is expected an increase of the impact of magnetic structures in the understanding of the electronic structure of materials with important functional properties.

- **Thin films**
- **Multiferroics and magnetoelectrics**
- **Superconductors**
- **Thermoelectrics and magnetocalorics**
- **Topological insulators**
- **Frustrated magnets**
- **...**

1. Historical introduction to neutron diffraction
2. Early Magnetic Crystallography. Shubnikov Groups and Representations
3. Impact of magnetic structures in condensed matter physics and chemistry
- 4. Future of Magnetic Crystallography. Superspace groups and Representations. New computing tools**



The (magnetic) structure of crystalline solids possess always a series of geometrical transformations that leave invariant the atomic (spin) arrangement.

These transformations constitute a **symmetry group** in the mathematical sense: point groups, space groups, Shubnikov groups, spin groups, superspace groups, ...



Pim de Wolff (1919–1998),
Delft Institute of Technology,
The Nederland

The introduction of
superspace approach was
a breakthrough that
allowed to treat “aperiodic
crystals” diffraction data



Seminal papers on superspace approach

Wolff, P. M. de (1974). *Acta Cryst.* **A30**, 777-785.

Wolff, P. M. de (1977). *Acta Cryst.* **A33**, 493-497.

Wolff, P. M. de, Janssen, T.
& Janner, A. (1981). *Acta Cryst.* **A37**, 625-636.

Acta Crystallographica Section B
Structural Science,
Crystal Engineering
and Materials

ISSN 2052-5206

Aperiodic crystals and superspace concepts

T. Janssen* and A. Janner

Theoretical Physics, University of Nijmegen,
Nijmegen, The Netherlands

Correspondence e-mail: t.janssen@science.ru.nl

For several decades the lattice periodicity of crystals, as shown by Laue, was considered to be their essential property. In the early sixties of the last century compounds were found which for many reasons should be called crystals, but were not lattice periodic. This opened the field of aperiodic crystals. An overview of this development is given. Many materials of this kind were found, sometimes with very interesting properties. In the beginning the development was slow, but the number of structures of this type increased enormously. In the meantime hundreds of scientists have contributed to this field using a multi-disciplinary approach.

Received 12 June 2014

Accepted 24 June 2014

Awarded with the **tenth Ewald Prize for “the development of superspace crystallography and its application to the analysis of aperiodic crystals” (Montreal 2014)**

PHYSICAL REVIEW B

VOLUME 30, NUMBER 3

1 AUGUST 1984

Superspace groups and Landau theory.

A physical approach to superspace symmetry in incommensurate structures

J. M. Pérez-Mato, G. Madariaga, and M. J. Tello

Departamento de Física, Facultad de Ciencias, Universidad del País Vasco, Apartado 644, Bilbao, Spain

(Received 19 December 1983)

Magnetic space and superspace groups, representation analysis: competing or friendly concepts?

Acta Cryst **A66**, 649 (2010)

Václav Petříček,* Jiří Fuxa and Michal Dušek

Institute of Physics of the Academy of Sciences of the Czech Republic, v.v.i., Na Slovance 2,
182 21 Praha 8, Czech Republic. Correspondence e-mail: petricek@fzu.cz

PHYSICAL REVIEW B

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(Received 19 December 1983)

Physica 126A (1984) 163–176
North-Holland, Amsterdam

**SUPERSPACE GROUPS AND REPRESENTATIONS OF ORDINARY
SPACE GROUPS: ALTERNATIVE APPROACHES TO THE
SYMMETRY OF INCOMMENSURATE CRYSTAL PHASES***

T. JANSSEN and A. JANNER

*Institute for Theoretical Physics, University of Nijmegen, Toernooiveld, 6525 ED Nijmegen,
The Netherlands*

Journal of Physics: Condensed Matter **24**, 163201 (2012)

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J. Phys.: Condens. Matter **24** (2012) 163201 (20pp)

[doi:10.1088/0953-8984/24/16/163201](https://doi.org/10.1088/0953-8984/24/16/163201)

TOPICAL REVIEW

Magnetic superspace groups and symmetry constraints in incommensurate magnetic phases

J M Perez-Mato¹, J L Ribeiro², V Petricek³ and M I Aroyo¹

The future of Magnetic Crystallography is clearly an unified approach of symmetry invariance and representations:

$$C3 > C0 + C1 + C2$$

$$\mathbf{r}_{l\mu} = \mathbf{l} + \mathbf{r}_{\mu} \quad x_4 = \mathbf{k} \mathbf{r}_{l\mu}$$

$$\mathbf{M}_{\mu}(x_4) = \mathbf{M}_{\mu,0} + \sum_n [\mathbf{M}_{\mu,ns} \sin(2\pi n x_4) + \mathbf{M}_{\mu,nc} \cos(2\pi n x_4)]$$

$$(\mathbf{R}, \theta | \mathbf{t}) \in \Omega_b \quad \theta = -1(\text{time reversal}) \quad \theta = 1(\text{otherwise})$$

The application of $(\mathbf{R}, \theta | \mathbf{t})$ operation to the modulated structure change the structure to another one with the modulation functions changed by a translation in the fourth coordinate

$$\mathbf{M}'_{\mu} = \mathbf{M}_{\mu}(x_4 + \tau)$$

The original structure can be recovered by a translation in the internal space and one can introduce a symmetry operator

$$(\mathbf{R}, \theta | \mathbf{t}, \tau)$$

If $(\mathbf{R}, \theta | \mathbf{t}, \tau)$ belongs to the (3+1)-dim superspace group of an incommensurate magnetic phase, the action of $\mathbf{R}$ on its propagation vector $\mathbf{k}$ necessarily transforms this vector into a vector equivalent to either $\mathbf{k}$ ($R_I = +1$) or $-\mathbf{k}$ ($R_I = -1$).

$$\mathbf{k} \cdot \mathbf{R} = R_I \mathbf{k} + \mathbf{H}_R$$

$\mathbf{H}_R$ is a reciprocal lattice vector of the basic structure and is different of zero only if $\mathbf{k}$ contains a commensurate component.

If in the basic structure $(\mathbf{R} | \mathbf{t})\mathbf{r}_\nu = \mathbf{r}_\mu + \mathbf{l}$ their atomic modulation functions are not independent and should verify

$$\mathbf{M}_\mu(R_I x_4 + \tau_0 + \mathbf{H}_R \mathbf{r}_\nu) = \theta \det(\mathbf{R}) \mathbf{R} \mathbf{M}_\nu(x_4)$$

$$\mathbf{u}_\mu(R_I x_4 + \tau_0 + \mathbf{H}_R \mathbf{r}_\nu) = \mathbf{R} \mathbf{u}_\nu(x_4)$$

$$\tau_0 = \tau + \mathbf{k} \mathbf{t}$$

The operators of the **magnetic superspace groups** are the same as those of **superspace groups** just extended with the time inversion label θ

The operators of the form: $(\mathbf{1}, +1 | \mathbf{t}, -\mathbf{k} \mathbf{t})$ constitute the lattice of the (3+1)-dim superspace group

The basic lattice translations are:

$$(\mathbf{1}, +1 | 100, -k_x), (\mathbf{1}, +1 | 010, -k_y), (\mathbf{1}, +1 | 001, -k_z), (\mathbf{1}, +1 | 000, 1)$$

Using the above basis we can define 3+1 symmetry operators of the form:

$$(\mathbf{R}, \theta | \mathbf{t}, \tau) \rightarrow (\mathbf{R}_S, \theta | \mathbf{t}_S) \quad \mathbf{t} = (t_1, t_2, t_3) \quad \tau_0 = \tau + \mathbf{k} \mathbf{t}$$

$$\mathbf{R}_S = \begin{pmatrix} R_{11} & R_{12} & R_{13} & 0 \\ R_{21} & R_{22} & R_{23} & 0 \\ R_{31} & R_{32} & R_{33} & 0 \\ H_{R1} & H_{R2} & H_{R3} & R_I \end{pmatrix} \quad \mathbf{t}_S = (t_1, t_2, t_3, \tau_0)$$

Simplified Seitz symbols for 3+1 symmetry operators

$$(\mathbf{R}, \theta | \mathbf{t}, \tau) \rightarrow (\mathbf{R}_s, \theta | \mathbf{t}_s) \quad \mathbf{t}_s = (t_1, t_2, t_3, \tau_0) \quad \tau_0 = \tau + \mathbf{k}\mathbf{t}$$

$$(\mathbf{R}, \theta | \mathbf{t}, \tau) \rightarrow \{\mathbf{R}, \theta | t_1 t_2 t_3 \tau_0\} \rightarrow \{\mathbf{R} | t_1 t_2 t_3 \tau_0\} \text{ or } \{\mathbf{R}' | t_1 t_2 t_3 \tau_0\}$$

Example: $(\mathbf{R}, \theta | 00 \frac{1}{2}, \frac{1}{2} - \frac{1}{2} \gamma) \rightarrow \{\mathbf{R}, \theta | 00 \frac{1}{2} \frac{1}{2}\} \quad \text{with } \mathbf{k} = \gamma \mathbf{c}^*$

Simple example

$$\bar{P}11'(\alpha\beta\gamma)0s$$

$$\{1 | 0000\} \quad x_1, x_2, x_3, x_4, +1$$

$$\{\bar{1} | 0000\} \quad -x_1, -x_2, -x_3, -x_4, +1$$

$$\{1' | 0001/2\} \quad x_1, x_2, x_3, x_4 + 1/2, -1$$

$$\{\bar{1}' | 0001/2\} \quad -x_1, -x_2, -x_3, -x_4 + 1/2, -1$$



Simplified magnetic structure factor in the superspace description with the notation used in **JANA-2006**

$$\mathbf{r}_{l\mu} = \mathbf{l} + \mathbf{r}_{\mu} \quad x_4 = \mathbf{k} \cdot \mathbf{r}_{l\mu}$$

$$\mathbf{M}_{\mu}(x_4) = \mathbf{M}_{\mu,0} + \sum_n [\mathbf{M}_{\mu,ns} \sin(2\pi n x_4) + \mathbf{M}_{\mu,nc} \cos(2\pi n x_4)]$$

$$\mathbf{F}_{mag}(\mathbf{H} \pm m\mathbf{k}) = p \sum_{\mu=1}^n f_{\mu}(|\mathbf{H} \pm m\mathbf{k}|) T(\mathbf{H} \pm m\mathbf{k}) \frac{\mathbf{M}_{\mu,mc} \pm i\mathbf{M}_{\mu,ms}}{2} \exp\{2\pi i \mathbf{H} \cdot \mathbf{r}_{\mu}\}$$

Simplified magnetic structure factor in the C2-b description used in **FullProf** (with notations adapted to those used in superspace approach)

$$\mathbf{M}_{l\mu} = \sum_{\{\mathbf{k}\}} \mathbf{S}_{\mathbf{k}\mu} \exp\{-2\pi i \mathbf{k} \cdot \mathbf{l}\} = \sum_{\{\mathbf{k}\}} \mathbf{M}_{\mathbf{k}\mu} \exp\{-2\pi i \mathbf{k} \cdot \mathbf{r}_{l\mu}\}$$

$$\mathbf{S}_{\mathbf{k}\mu} = \frac{1}{2} (\mathbf{R}_{\mathbf{k}\mu} + i \mathbf{I}_{\mathbf{k}\mu}) \exp\{-2\pi i \phi_{\mathbf{k}}\} = \frac{1}{2} (\mathbf{M}_{\mathbf{k}\mu,c} + i \mathbf{M}_{\mathbf{k}\mu,s}) \exp\{-2\pi i \mathbf{k} \cdot \mathbf{r}_{\mu}\}$$

$$\mathbf{M}(\mathbf{h}) = p \sum_{\mu=1}^n f_{\mu}(h) T_{\mu} \mathbf{S}_{\mathbf{k}\mu} \exp\{2\pi i (\mathbf{H} + \mathbf{k}) \cdot \mathbf{r}_{\mu}\}$$

$$\mathbf{M}(\mathbf{h}) = \frac{1}{2} p \sum_{\mu=1}^n f_{\mu}(h) T_{\mu} (\mathbf{M}_{\mathbf{k}\mu,c} + i \mathbf{M}_{\mathbf{k}\mu,s}) \exp\{2\pi i \mathbf{H} \cdot \mathbf{r}_{\mu}\}$$

Most used programs for Magnetic Structure determination and refinement

Commensurate structures only: **GSAS**, **RIETAN**
TOPAS symmetry modes

General magnetic structures:

Single Crystals only: **MAGLSQ** (CCSL)

Single Crystal and Powders: **FullProf**, **JANA-2006**

In red, we have emphasized the programs with strong active projects for developing new methods for magnetic structures



A series of computing tools for crystallography including magnetic structures are available at Bilbao Crystallographic Server

bilbao crystallographic server

[The crystallographic site at the Condensed Matter Physics Dept. of the University of the Basque Country]

[Space Groups] [Layer Groups] [Rod Groups] [Frieze Groups] [Wyckoff Sets]



IYCr2014

2014: International Year of Crystallography

NEW!

Satellite workshop of the 2014 IUCr Congress:

Role of Magnetic Symmetry in the Description and Determination of Magnetic Structures.
Hamilton, Canada
14-16 August 2014

Space Groups Retrieval Tools

GENPOS	Generators and General Positions of Space Groups
WYCKPOS	Wyckoff Positions of Space Groups
HKLCD	Reflection conditions of Space Groups
MAXSUB	Maximal Subgroups of Space Groups
SERIES	Series of Maximal Isomorphic Subgroups of Space Groups
WYCKSETS	Equivalent Sets of Wyckoff Positions
NORMALIZER	Normalizers of Space Groups
KVEC	The k-vector types and Brillouin zones of Space Groups
SYMMETRY OPERATIONS	Geometric interpretation of matrix column representations of symmetry operations
IDENTIFY GROUP 	Identification of a Space Group from a set of generators in an arbitrary setting

Magnetic Symmetry and Applications

MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
MAGNEXT	Extinction Rules of Magnetic Space Groups
IDENTIFY MAGNETIC GROUP ⚠	Identification of a Magnetic Space Group from a set of generators in an arbitrary setting
MAXMAGN ⚠	Maximal magnetic space groups for a given a propagation vector and resulting magnetic structural models
k-SUBGROUPSMAG ⚠	Magnetic subgroups consistent with some given propagation vector(s) or a supercell
MAGNDATA ⚠	A collection of magnetic structures with transportable cif-type files

Structure Utilities

CELLTRAN	Transform Unit Cells
STRAIN	Strain Tensor Calculation
WPASSIGN	Assignment of Wyckoff Positions
TRANSTRU	Transform structures.
SETSTRU ⚠	Alternative Settings for a given Crystal Structure
EQUIVSTRU	Equivalent Descriptions for a given Crystal Structure
STRCONVERT	Convert & Edit Structure Data (supports the CIF, mCIF, VESTA, VASP formats -- with magnetic information where available)
VISUALIZE	Visualize structures using Jmol
COMPSTRU ⚠	Comparison of Crystal Structures with the same Symmetry
STRUCTURE RELATIONS ⚠	Evaluation of structure relationships [transformation matrix] between group-subgroup related phases
PSEUDOLATTICE	Pseudosymmetry of a lattice and compatible supergroups

ISOTROPY Software Suite

Harold T. Stokes, Dorian M. Hatch, and Branton J. Campbell, Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84606, USA, stokesh@byu.edu

Description: The ISOTROPY software suite is a collection of software which applies group theoretical methods to the analysis of phase transitions in crystalline solids.

How to cite: ISOTROPY Software Suite, iso.byu.edu.

References and Resources

Isotropy subgroups and distortions

- **ISODISTORT:** Explore and visualize distortions of crystalline structures. Possible distortions include atomic displacements, atomic ordering, strain, and magnetic moments.
- **ISOSUBGROUP:** Coming soon!
- **ISOTROPY:** Interactive program using command lines to explore isotropy subgroups and their associated distortions.
- **SMODES:** Find the displacement modes in a crystal which brings the dynamical matrix to block-diagonal form, with the smallest possible blocks.
- **FROZSL:** Calculate phonon frequencies and displacement modes using the method of frozen phonons.

Space groups and irreducible representations

- **ISOCIF:** Create or modify CIF files.
- **FINDSYM:** Identify the space group of a crystal, given the positions of the atoms in a unit cell.
- **New! ISO-IR:** Tables of Irreducible Representations. The 2011 version of IR matrices.
- **ISO-MAG:** Tables of magnetic space groups, both in human-readable and computer-readable forms.

Superspace Groups

- **ISO(3+d)D:** (3+d)-Dimensional Superspace Groups for $d=1,2,3$
- **ISO(3+1)D:** Isotropy Subgroups for Incommensurately Modulated Distortions in Crystalline Solids: A Complete List for One-Dimensional Modulations
- **FINDSSG:** Identify the superspace group symmetry given a list of symmetry operators.
- **TRANSFORMSSG:** Transform a superspace group to a new setting.

Phase Transitions

- **COPL:** Find a complete list of order parameters for a phase transition, given the space-group symmetries of the parent and subgroup phases.
- **INVARIANTS:** Generate invariant polynomials of the components of order parameters.
- **COMSUBS:** Find common subgroups of two structures in a reconstructive phase transition

Linux

- **ISOTROPY Software Suite for Linux:** includes ISOTROPY, FINDSYM, SMODES, COMSUBS.

ISOTROPY Software Suite

Harold T. Stokes, Dorian M. Hatch, and Branton J. Campbell, Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84606, USA, stokes@byu.edu

Description: The ISOTROPY software suite is a collection of software which applies group theoretical methods to the analysis of phase transitions in crystalline solids.

How to cite: ISOTROPY Software Suite, iso.byu.edu.

References

A huge amount of work on symmetry has been developed by Harold Stokes, Dorian Hatch and Branton Campbell. Stokes developed ISOTROPY and many algorithms for working with space groups and representations. Together with the programs they have made available databases to be used by external software

- **FINDSYM:** Identify the
- **New! ISO-IR:** Tables of
- **ISO-MAG:** Tables of

Superspace Groups

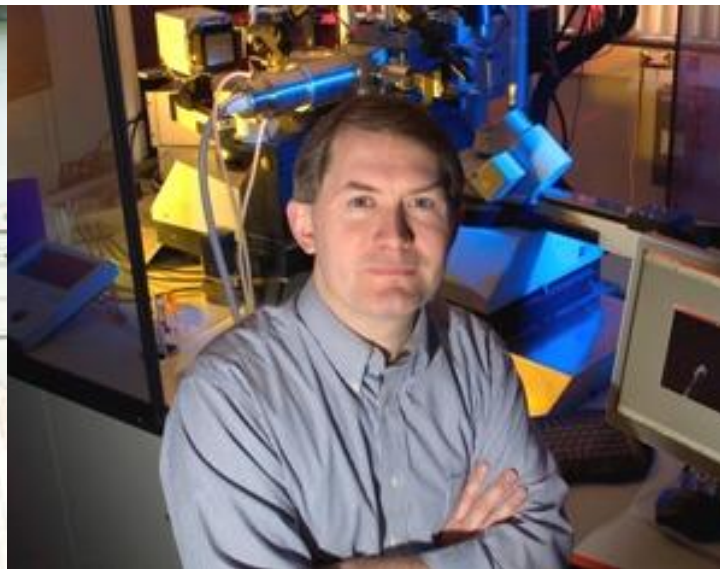
- **ISO(3+d)D:** (3+d)-D
- **ISO(3+1)D:** Isotropy
- **FINDSSG:** Identify the
- **TRANSFORMSSG:**

Phase Transition

- **COPL:** Find a comp
- **INVARIANTS:** Gene
- **COMSUBS:** Find co

Linux

- **ISOTROPY Software**



lations



IUCr Commission on Magnetic Structures

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IUCr Commission on Magnetic Structures

The Commission on Magnetic Structures (CMS) was established *ad interim* by the Executive Committee in January 2011 and confirmed at the Madrid General Assembly in August 2011. Its primary purpose is to facilitate research on the discovery and communication of magnetic structures in magnetically ordered materials; and its present focus is to cultivate a community consisting of interested participants from diverse fields of research, who can establish standards for defining and communicating the crystallographic details of magnetic structures. The scope of the Commission's consideration encompasses a broad range of magnetic structure types, including commensurate magnetic structures, modulated and otherwise aperiodic magnetic structures, low-dimensional magnetic structures, disordered magnetic structures, etc.

The commission's terms of reference are as follows:

- Establish standards for the description and dissemination of magnetic structures and their underlying symmetries (representations of propagation vector group, 'complete' representation of the group necessary for multi- k structures, 3D magnetic Shubnikov space groups, superspace symmetry ...), and promote these standards within the IUCr and among other research communities that rely on magnetic structure information.

Chair

Prof. Branton J. Campbell

Members

Prof. Jane Brown

Prof. Daniel B. Litvin

Dr. Vaclav Petricek

Prof. Alexander N. Pirogov

Dr. Vladimir Pomjakushin

Dr. Juan Rodriguez-Carvajal

Prof. Taku J Sato

Prof. Wieslawa Sikora

Consultants

Prof. Mois I. Aroyo

Dr. M. Teresa Fernandez-Diaz

Prof. J. Manuel Perez-Mato

Prof. Harold T. Stokes

CrysFML: open Crystallographic Library in F90 at
<https://forge.epn-campus.eu/projects/crysfml>

As a result of the availability of new databases I have developed new tools to be used within the FullProf Suite

Mag_Info:	information on Shubnikov groups
mCIF_to_PCR:	conversion of mCIF files to PCR files for FullProf

FullProf exports (for commensurate structures) an mCIF file that can be read by **ISOCIF** and the Bilbao Crystallographic Server



CrysFML

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Overview

Crystallographic Fortran 95 Modules Library

- Licence: LGPL

Issue tracking

- **Bug:** 2 open / 2
- **Feature:** 7 open / 7
- **Support:** 0 open / 0

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 Reporter: **Fischer, Henry, Hutanu, Vladimir, Mutti, Paolo, Nénert, Gwilherm**

Latest news

CrysFML License

CrysFML is now distributed under the Lesser GNU Public License
 Added by **Rodriguez-Carvajal, Juan** almost 2 years ago

New files in CrysFML/Src/CFML (default for Intel compiler)

Added by **Rodriguez-Carvajal, Juan** almost 5 years ago

How to download the whole CrysFML repository

The use of a GUI for SVN and the steps for creating a local copy of the repository is shortly explained
 Added by **Rodriguez-Carvajal, Juan** almost 5 years ago

CrysFML

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root

[Statistics](#) | Revision:

Name	Size	Revision	Age	Author	Comment
 Help		930	about 1 month	angel, ross	Updated hnd help file with changes to point_group
 Html		477	about 3 years	Gonzalez Platas, Javier	Updating the Documentation
 Program_Examples		935	30 days	Rodriguez-Carvajal, Juan	Changing the name of one of the crystal calcula...
 Scripts		932	30 days	Bytchkov, Aleksei	adding keyword 'deb' to makecrys
 Src		936	25 days	Bytchkov, Aleksei	debugging ref_codes for molecular crystals
 cmake		884	5 months	Rodriguez-Carvajal, Juan	Adding heap-arrays in set_compiler_flags.cmake ...
 CMakeLists.txt	2.8 kB	804	9 months	Rodriguez-Carvajal, Juan	Updating a CMakeLists.txt file and changing com...
 README	3.7 kB	569	over 2 years	Pellegrini, Eric	Removed unused files

svn:ignore: Intel Lahey gfortran build G95 script.bat *.project ifort .cproject

Latest revisions

#	Date	Author	Comment
936 	15/07/2014 10:27 am	Bytchkov, Aleksei	debugging ref_codes for molecular crystals
935  	10/07/2014 03:44 pm	Rodriguez-Carvajal, Juan	Changing the name of one of the crystal calculators programs to avoid clashes.
934  	10/07/2014 03:21 pm	Rodriguez-Carvajal, Juan	Changes for using VarF(5) as indicator to restrict the calculation of the BVS global instability index to a series of atoms. Still not tested
933  	10/07/2014 01:21 pm	Bytchkov, Aleksei	overloading of the write_cfl subroutine for molecular crystals moving write_cfl into CFML_IO_Formats module
932  	10/07/2014 11:23 am	Bytchkov, Aleksei	adding keyword 'deb' to makecrys
931  	10/07/2014 11:21 am	Bytchkov, Aleksei	changes to the make_crysFML to avoid problems with 132 char limits with GFortran
930  	04/07/2014 04:57 pm	angel, ross	Updated hnd help file with changes to point_group
929  	03/07/2014 08:34 pm	Gonzalez Platas, Javier	Documentation for CrysFML
928  	03/07/2014 03:50 pm	Roisnel, Thierry	Cryscal_TR folder has been removed and replaced by CRYSCALc one (CRYSCAL has been renamed as CRYSCALc)
927 	03/07/2014 03:40 pm	Roisnel, Thierry	CRYSCAL has been renamed as CRYSCALc

CrysFML

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root / Program_Examples

Statistics | Revision:

Name	Size	Revision	Age	Author	Comment
 CRYSCALc		927	about 1 month	Roisnel, Thierry	CRYSCAL has been renamed as CRYSCALc
 Cryst_calculator_console		935	30 days	Rodriguez-Carvajal, Juan	Changing the name of one of the crystal calcula...
 Faults		912	about 1 month	Rodriguez-Carvajal, Juan	Correcting a bug in Faults_Read.f90: the values...
 Magnetism		924	about 1 month	Rodriguez-Carvajal, Juan	Updating CFML_MagSymm.f90 and magref.f90 ... No...
 Metrics		885	5 months	Rodriguez-Carvajal, Juan	Changes in Cryst_calculator_console for allowin...
 Miscellaneous		907	2 months	Rodriguez-Carvajal, Juan	Changes in Data_Articles_Mod.f90 and ILL_Pubs_W...
 PowderPattern		880	5 months	Rodriguez-Carvajal, Juan	Changes in various modules for improving the fo...
 SXTal_Diffractometry		758	over 1 year	Rodriguez-Carvajal, Juan	Updating the program d10_flat_cone. New options...
 Simbo-Enermag		896	3 months	Rodriguez-Carvajal, Juan	Minor changes in CFML_Optimization_LSQ.f90 and ...
 SpaceGroups		689	almost 2 years	Rodriguez-Carvajal, Juan	Updating some program examples and correcting s...
 StructureFactors		549	over 2 years	Rodriguez-Carvajal, Juan	Change in the directory structure of CrysFML: C...
 Structures_GlobalOptimization		934	30 days	Rodriguez-Carvajal, Juan	Changes for using VarF(5) as indicator to restr...
 Twins		885	5 months	Rodriguez-Carvajal, Juan	Changes in Cryst_calculator_console for allowin...
 XRFit		888	5 months	Rodriguez-Carvajal, Juan	Small change in Program_Examples/XRFit/cw_diff...
 cfml4c		425	over 3 years	Gonzalez Platas, Javier	Updating files
 hkl_gen		899	3 months	fabelrosa, oscarrramon	Small format changes in hkl_gen.f90

Latest revisions

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CrysFML

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[Statistics](#) | Revision:

Name	Size	Revision	Age	Author	Comment
 CRYSCALc		927	about 1 month	Roisnel, Thierry	CRYSCAL has been renamed as CRYSCALc
 Cryst_calculator_console		935	30 days	Rodriguez-Carvajal, Juan	Changing the name of one of the crystal calcula...
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Acknowledgements

Jane Brown for helping me at my arrival to the ILL in 1988 and being an example to follow

Juan Manuel Perez-Mato, Mois Aroyo, Branton Campbell for many discussions about symmetry

All the members of the **Diffraction Groups at ILL and LLB** for helping me to progress and making my working life pleasant and exciting

Acknowledgements (cont.)

All the **co-developers of the FullProf Suite:**

Thierry Roisnel, Javier Gonzalez-Platas, Oscar Baltuano,
Carlos Frontera, Laurent Chapon

All the **users of the FullProf Suite** for helping us to improve
our analytical tools

Thank you
for your kind attention