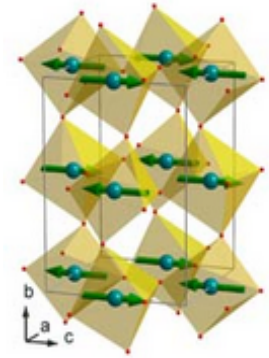
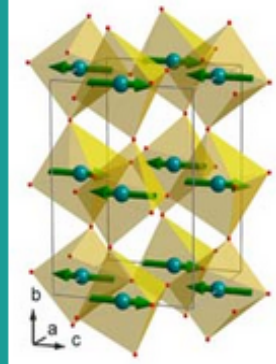
neutrons.ornl.gov/conf/2014/magstr/



Magnetic Structure Determination from Neutron Diffraction Data

June 5 – 8, 2014

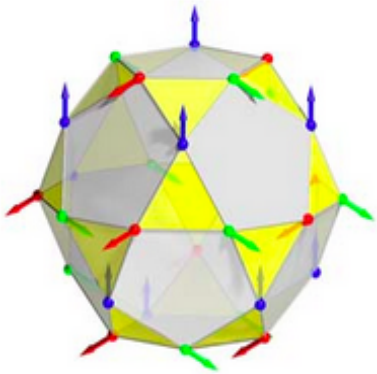


Oak Ridge National Laboratory — Oak Ridge, Tennessee, USA

About the School

http://www.mrs.org/acns-2014-satellite-meetings

The Magnetic Structure Determination Workshop 2014 aims to enhance the community studying magnetism in materials by learning from experts the essential theoretical foundations to magnetic representation analysis and work through real examples to gain experience in solving and refining magnetic structures from neutron powder and single crystal diffraction data.



Confirmed Speakers:

- Juan Rodríguez-Carvajal (ILL, Grenoble)
- William Ratcliff (NCNR)
- Ovidiu Garlea (ORNL)
- Clarina de la Cruz, (ORNL)
- Huibo Cao (ORNL)

Registration is now closed!

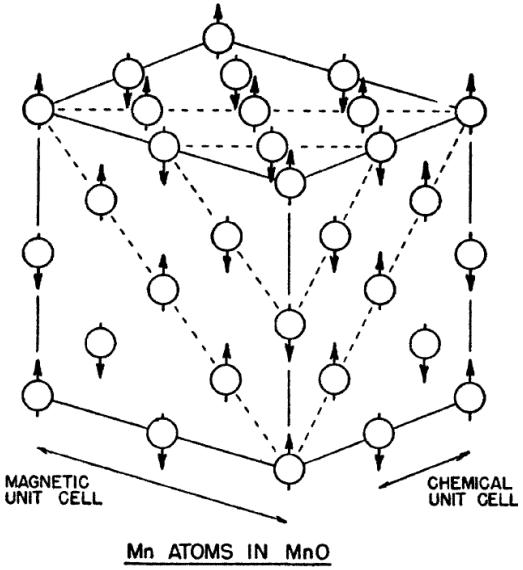
The workshop sessions will be held at Hilton Knoxville, 501 W Church Ave Knoxville, TN 37902. Participants are expected to arrange for their own travel, board, and lodging.

Physical Review 76, 1256–1257 (1949)

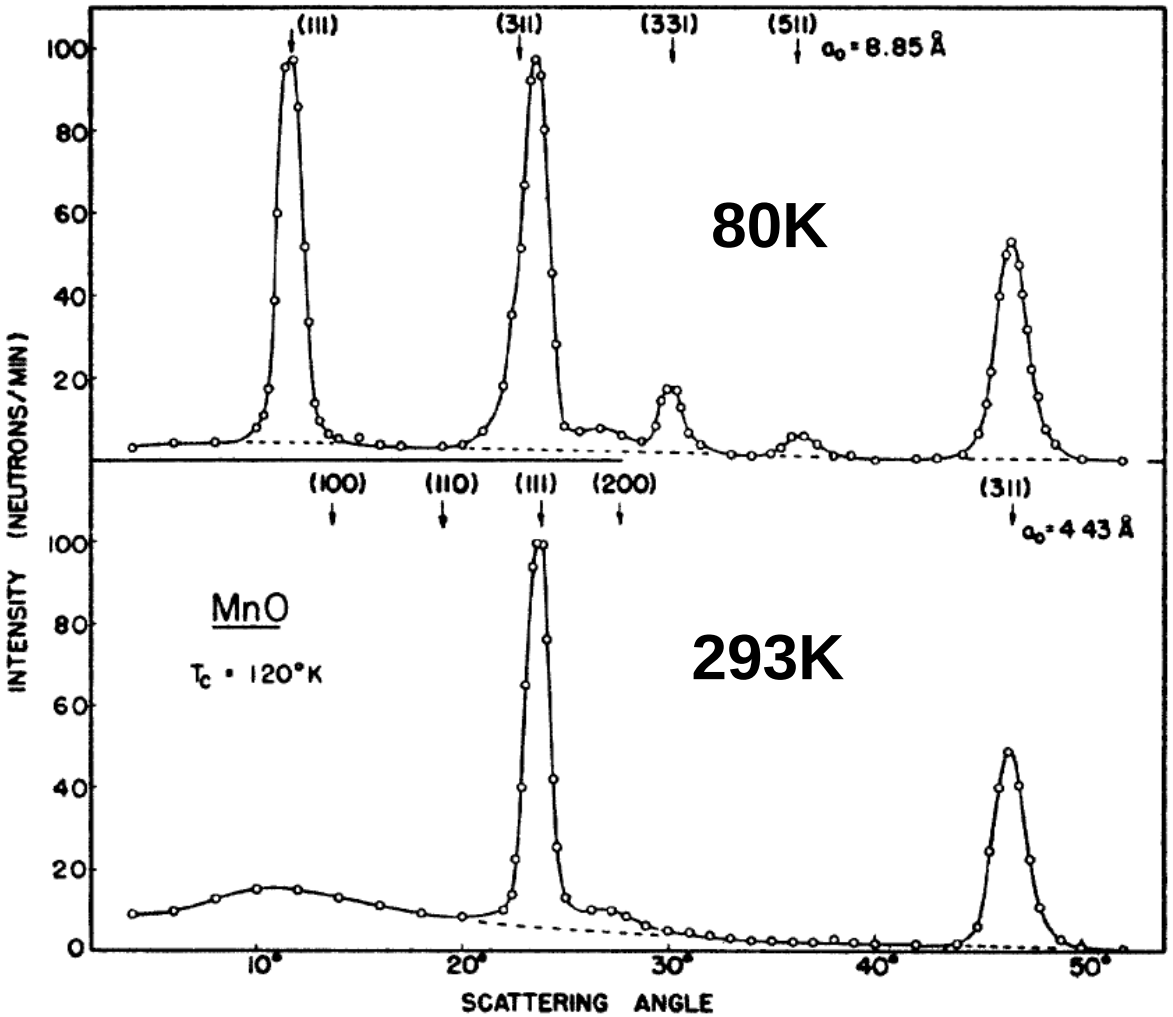
Detection of Antiferromagnetism by Neutron Diffraction

C. G. Shull
Oak Ridge National Laboratory, Oak Ridge, Tennessee
J. Samuel Smart
Naval Ordnance Laboratory, White Oak, Silver Spring, Maryland

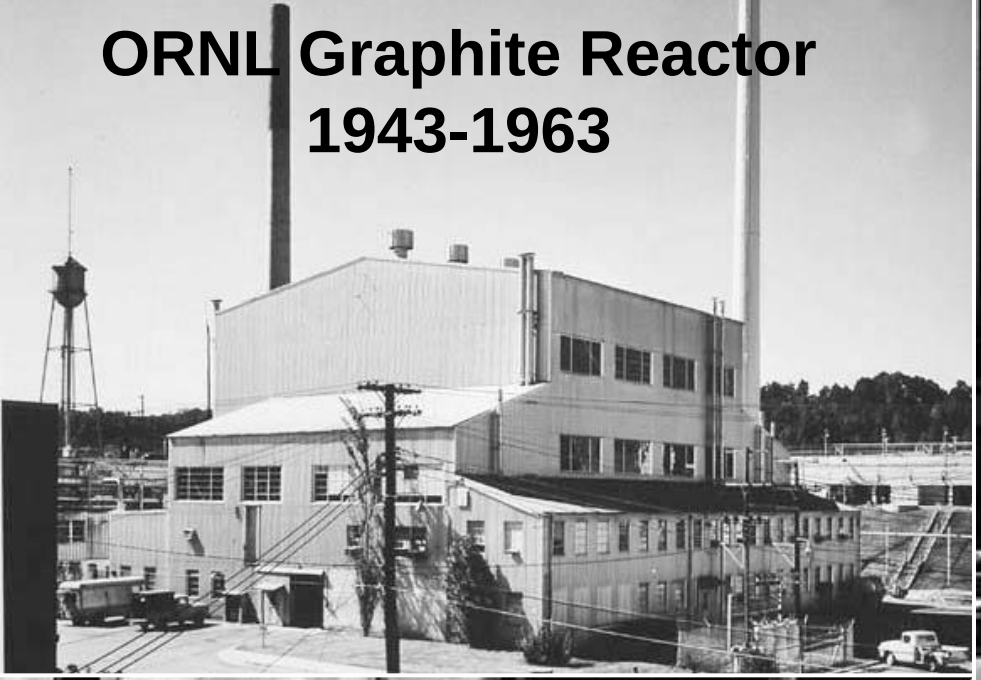
August 29, 1949

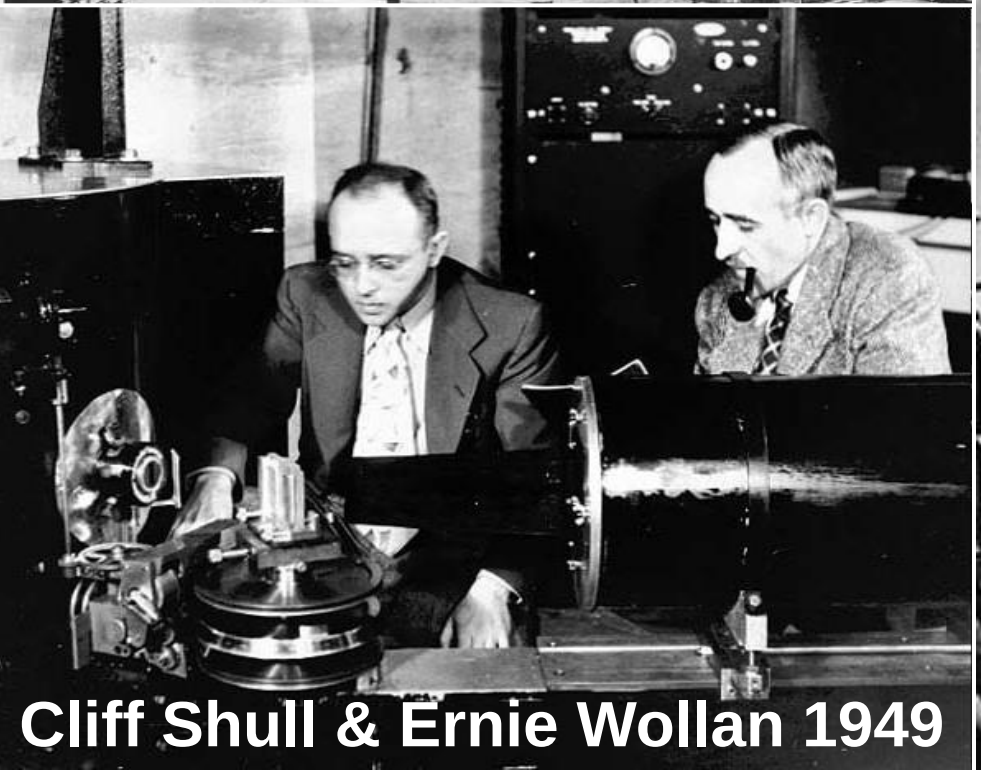


MnO
T_N = 120K

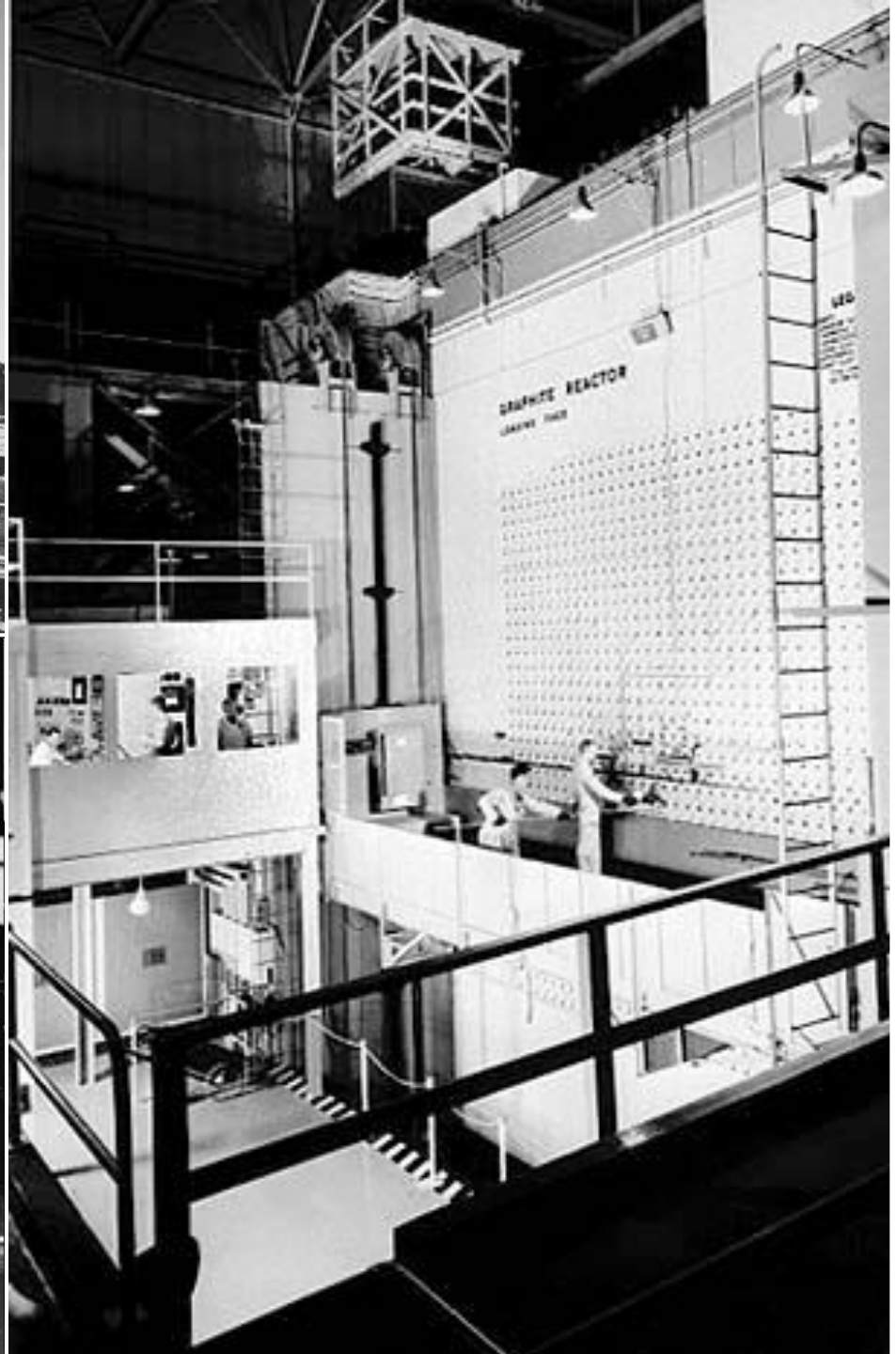


ORNL Graphite Reactor 1943-1963





Cliff Shull & Ernie Wollan 1949



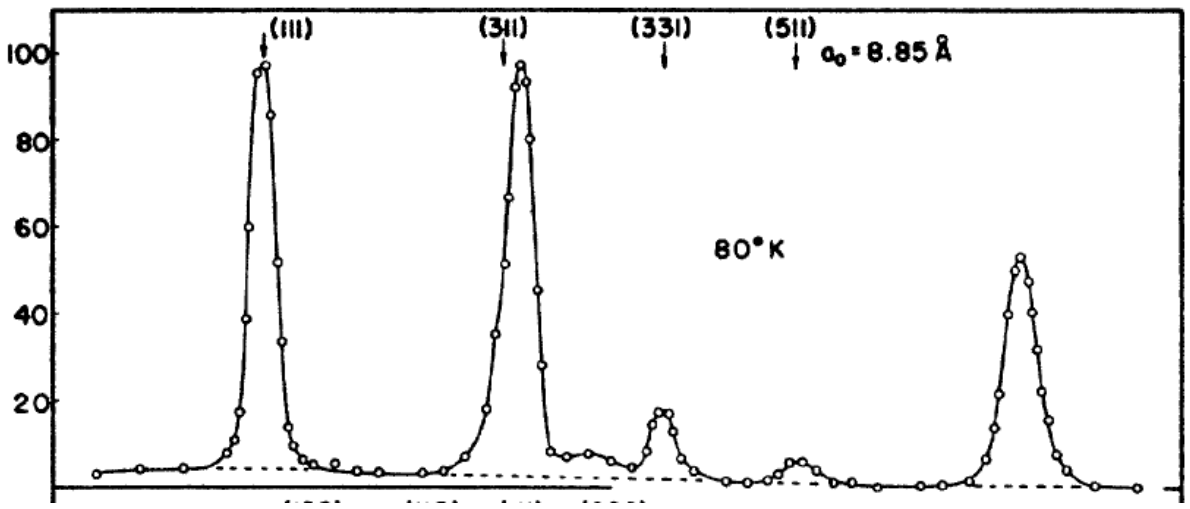
PHYSICAL REVIEW VOLUME 83, NUMBER 2 JULY 15, 1951

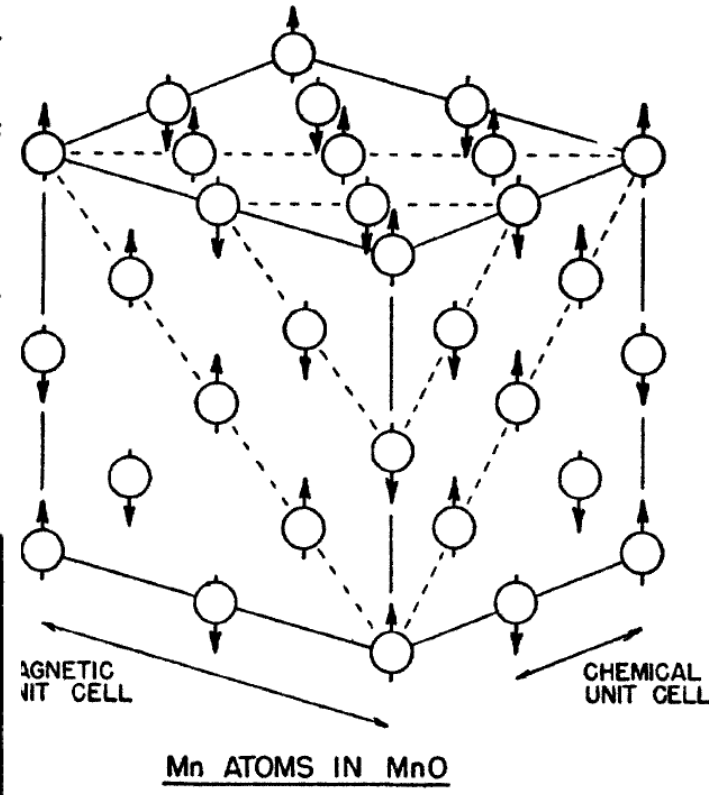
Neutron Diffraction by Paramagnetic and Antiferromagnetic Substances

C. G. SHULL, W. A. STRAUSER, AND E. O. WOLLAN
Oak Ridge National Laboratory, Oak Ridge, Tennessee
(Received March 2, 1951)

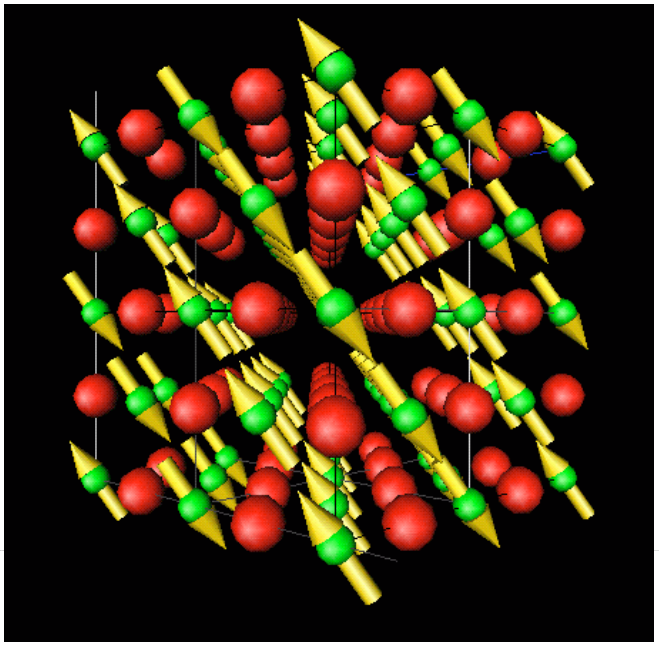
TABLE II. Comparison between observed MnO antiferromagnetic intensities and those calculated for various models of magnetic orientation with respect to crystallographic axes.

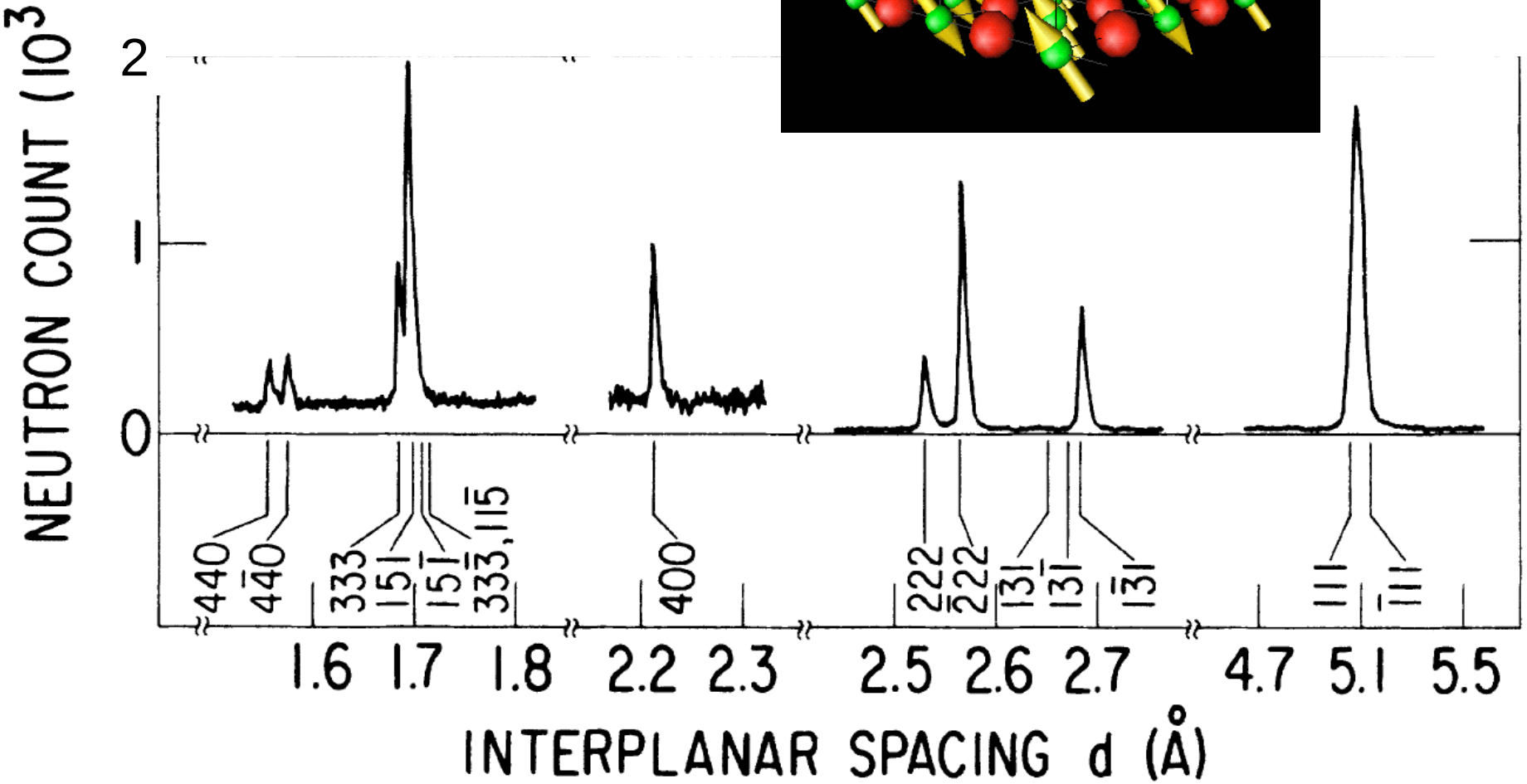
	(100) (a)	(111) (b)	⊥[111] (c)	Observed (neutrons/min)
(111)	1038	0	1560	1072
(311)	460	675	...	308
(331)	129	109	...	132
(511)} (333)}	54	24	...	70

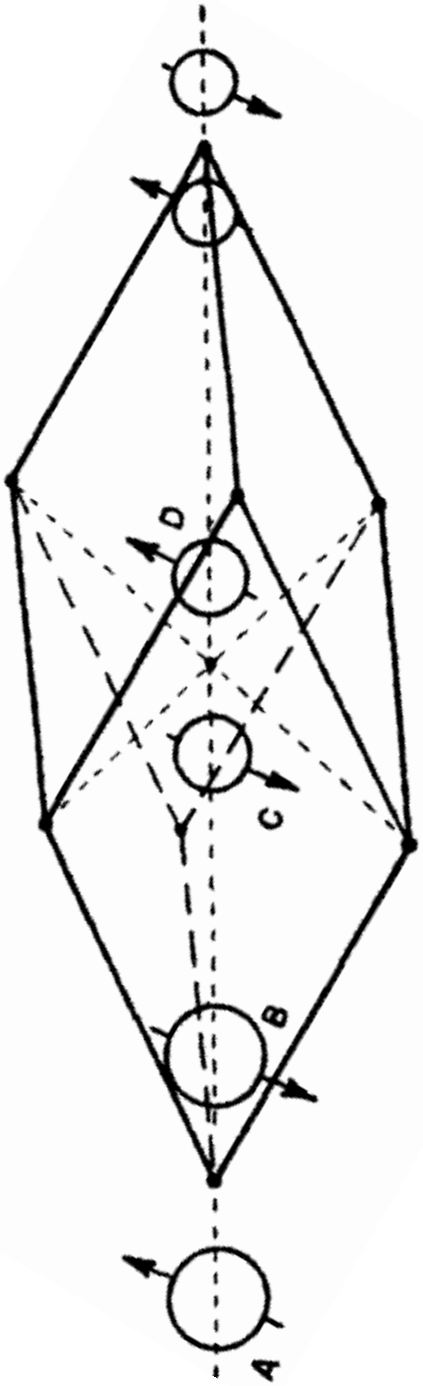


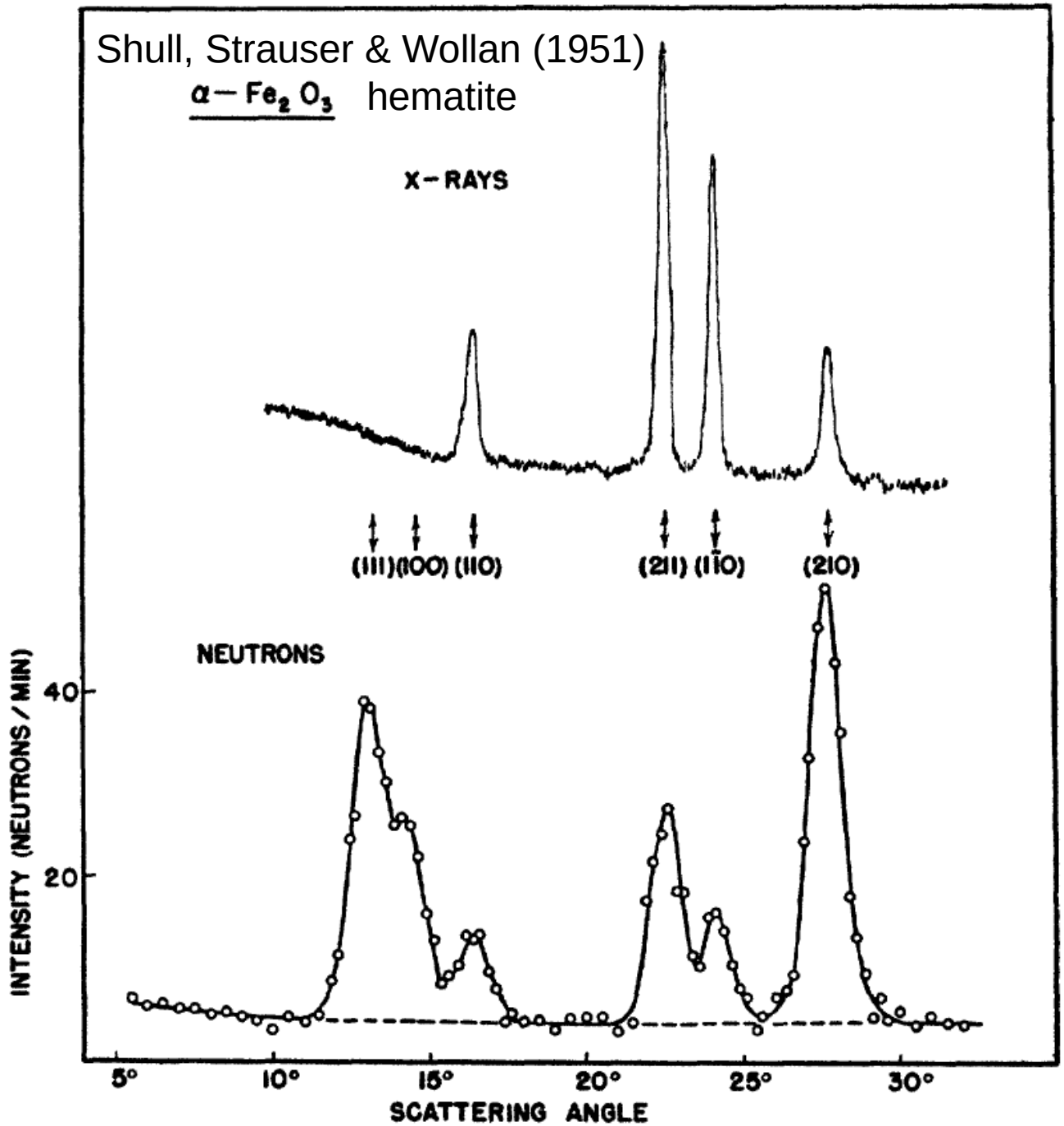


H. Shaked, J. Faber, Jr., R.L. Hitterman, Low-temperature magnetic structure of MnO: A high-resolution neutron-diffraction study. Phys. Rev. B (1988) 38, 11901-11903.

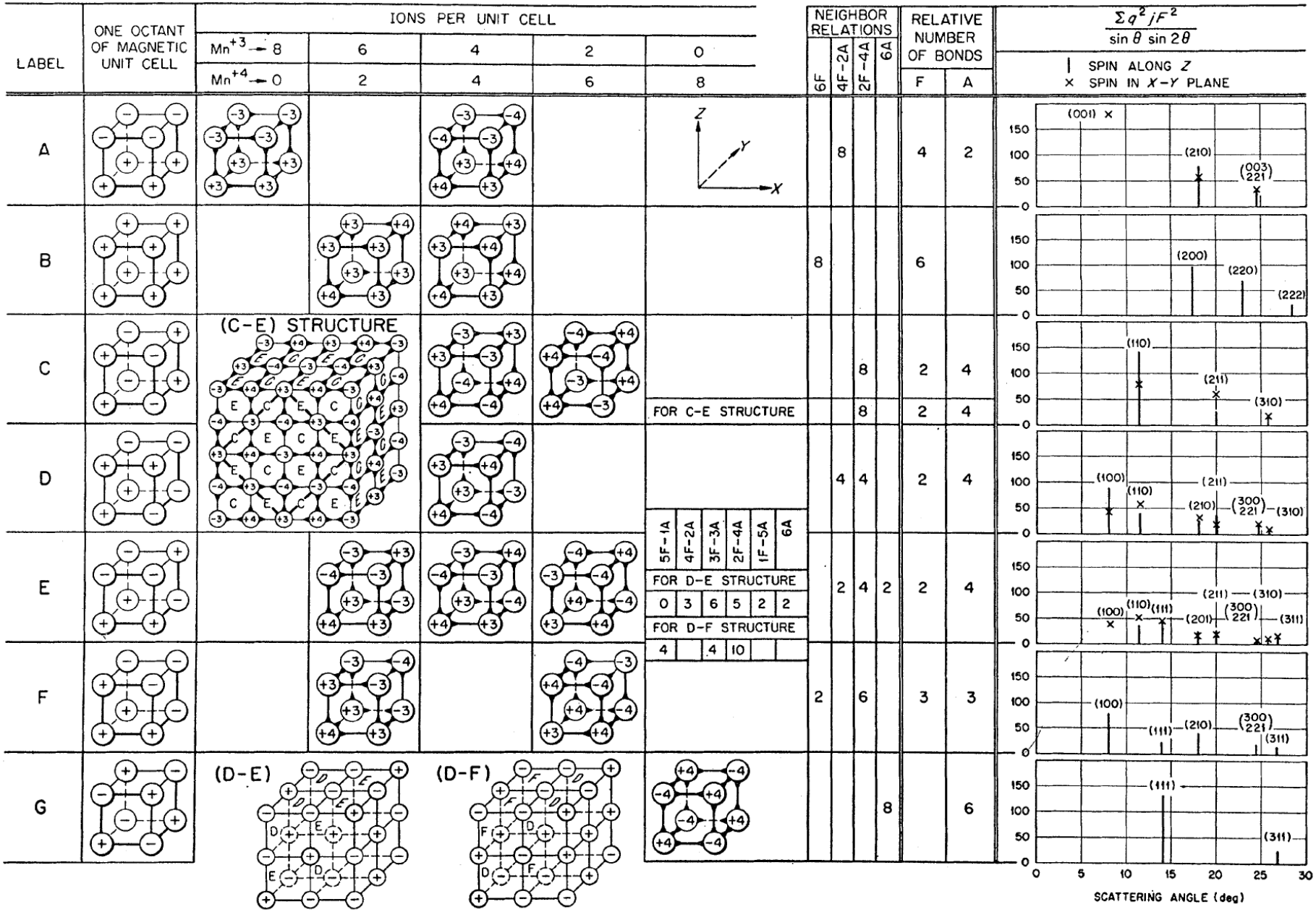





D
C
B
A


Shull, Strauser & Wollan (1951)
α – Fe2 O3 hematite
X – RAYS
(111) (100) (110)
(211) (1̄10)
(210)
NEUTRONS
INTENSITY (NEUTRONS / MIN)
40
20
5°
10°
15°
20°
25°
30°
SCATTERING ANGLE

Wollan & Koehler Phys. Rev. 1955, 100(2), 545-563. $La_{1-x}Ca_xMnO_3$ magnetic structures



SNS Beam Line	Instrument Name	HFIR Beam Line	Instrument Name
1B	NOMAD Nanoscale-Ordered Materials Diffractometer	CG-1	Development Beam Line
2	BASIS Backscattering Spectrometer	CG-1D	IMAGING Neutron Imaging Prototype Facility
3	SNAP Spallation Neutrons and Pressure Diffractometer	CG-2	GP-SANS General-Purpose Small-Angle Neutron Scattering Diffractometer
4A	MR Magnetism Reflectometer	CG-3	Bio-SANS Biological Small-Angle Neutron Scattering Instrument
4B	LR Liquids Reflectometer	CG-4C	CTAX Cold Neutron Triple-Axis Spectrometer

5	CNCS Cold Neutron Chopper Spectrometer	CG-4D	Imagine Quasi-Laue diffractometer at HFIR
6	EQ-SANS Extended Q-Range Small-Angle Neutron Scattering Diffractometer	HB-1	PTAX Polarized Triple-Axis Spectrometer
7	VULCAN Engineering Materials Diffractometer	HB-1A	FIE-TAX Fixed-Incident-Energy Triple-Axis Spectrometer
11A	POWGEN Powder Diffractometer	HB-2A	Powder Neutron Powder Diffractometer
11B	MANDI Macromolecular Neutron Diffractometer	HB-2B[1]	NRSF2 Neutron Residual Stress Mapping Facility[1]
12	TOPAZ Single-Crystal Diffractometer	HB-2C	WAND US/Japan Wide-Angle Neutron

13	FNPB Fundamental Neutron Physics Beam Line	HB-3	TAX Triple-Axis Spectrometer
14B	HYSPEC HYSPEC—Hybrid Spectrometer	HB-3A	FC Four-Circle Diffractometer
15	NSE Neutron Spin Echo Spectrometer		
16B	VISION Vibrational Spectrometer		
17	SEQUOIA Fine-Resolution Fermi Chopper Spectrometer		
18	ARCS Wide Angular-Range Chopper Spectrometer		

Acta Cryst. (1968). A**24**, 217-231 [doi:10.1107/S0567739468000306]

Representation analysis of magnetic structures

E. F. Bertaut

Abstract: 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 **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 **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 **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^{16}_{2h}). We illustrate the physical context of representation theory by constructing an effective spin Hamiltonian *H* invariant under the crystallographic space group and under spin reversal. *H* is even in the spins and automatically invariant under the (isomorphous) magnetic group. We show by the example of CoO that the invariants in *H*, formed with the help of basis vectors, give information on the nature of spin coupling as for instance isotropic (Heisenberg-Néel) coupling, vectorial (Dzialoshinski-Moriya) and anisotropic symmetric couplings. Magnetic structures, cited in the text to show the implications of the representation theory of space groups are $ErFeO_3$, $ErCrO_3$, $TbFeO_3$, $TbCrO_3$, $DyCrO_3$, $YFeO_3$, V_2CaO_4, β-$CoSO_4$, Er_2O_3, CoO and RMn_2O_5 (R = Bi, Y or rare earth). Representation theory of *magnetic* groups must be considered when the Hamiltonian contains terms which are odd in the spins. The case may occur when the magnetic energy is coupled with other forms of energy as for instance in the field of magneto-electricity. Here again representation theory correctly predicts the couplings between magnetic and electric polarizations as shown on $LiCoPO_4$ and (previously) on $FeGaO_3$.

Acta Cryst. (2006). A**62**, 115-128 [doi:10.1107/S0108767305040286]

Bilbao Crystallographic Server. II. Representations of crystallographic point groups and space groups

M. I. Aroyo, A. Kirov, C. Capillas, J. M. Perez-Mato and H. Wondratschek

Abstract: The Bilbao Crystallographic Server is a web site with crystallographic programs and databases freely available on-line (http://www.cryst.ehu.es). The server gives access to general information related to crystallographic symmetry groups (generators, general and special positions, maximal subgroups, Brillouin zones *etc.*). Apart from the simple tools for retrieving the stored data, there are programs for the analysis of group-subgroup relations between space groups (subgroups and supergroups, Wyckoff-position splitting schemes *etc.*). There are also software packages studying specific problems of solid-state physics, structural chemistry and crystallography. This article reports on the programs treating representations of point and space groups. There are tools for the construction of irreducible representations, for the study of the correlations between representations of group-subgroup pairs of space groups and for the decompositions of Kronecker products of representations.

Keywords: Bilbao Crystallographic Server; point and space groups; representations of crystallographic groups.

J. Appl. Cryst. (2012). **45**, 1236-1247 [doi:10.1107/S0021889812042185]

Magnetic symmetry in the Bilbao Crystallographic Server: a computer program to provide systematic absences of magnetic neutron diffraction

S. V. Gallego, E. S. Tasci, G. de la Flor, J. M. Perez-Mato and M. I. Aroyo

Abstract: *MAGNEXT* is a new computer program available from the Bilbao Crystallographic Server (http://www.cryst.ehu.es) that provides symmetry-forced systematic absences or extinction rules of magnetic nonpolarized neutron diffraction. For any chosen Shubnikov magnetic space group, the program lists all systematic absences, and it can also be used to obtain the list of the magnetic space groups compatible with a particular set of observed systematic absences. Absences corresponding to specific ordering modes can be derived by introducing effective symmetry operations associated with them. Although systematic extinctions in neutron diffraction do not possess the strong symmetry-resolving power of those in nonmagnetic crystallography, they can be important for the determination of some magnetic structures. In addition, *MAGNEXT* provides the symmetry-adapted form of the magnetic structure factor for different types of diffraction vectors, which can then be used to predict additional extinctions caused by some prevailing orientation of the atomic magnetic moments. This program, together with a database containing comprehensive general information on the symmetry operations and the Wyckoff positions of the 1651 magnetic space groups, is the starting point of a new section in the Bilbao Crystallographic Server devoted to magnetic symmetry and its applications.

Keywords: magnetic nonpolarized neutron diffraction; systematic absences; extinction rules; Bilbao Crystallographic Server; *MAGNEXT*; computer programs.