Magnetic Structure Determination from Neutron Diffraction Data

21-23 October 2019
Shull Wollan Building
US/Eastern timezone

Administrative Support
Angie Woody
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865-574-8098

About the School

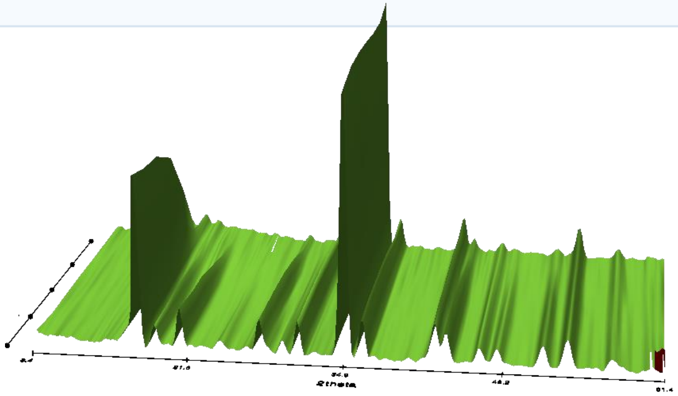
The school will provide hands-on training on how to determine magnetic structures from powder and single-crystal neutron data. The techniques of representational analysis and magnetic space groups will be introduced and used in a series of examples.

This school is a mini version of the Magnetic Structure Determination from Neutron Diffraction Data (Magstr) school and will be held at ORNL on the three days prior to the Pittsburgh Diffraction Conference, also held at ORNL that week. (https://conference.sns.gov/event/78/)

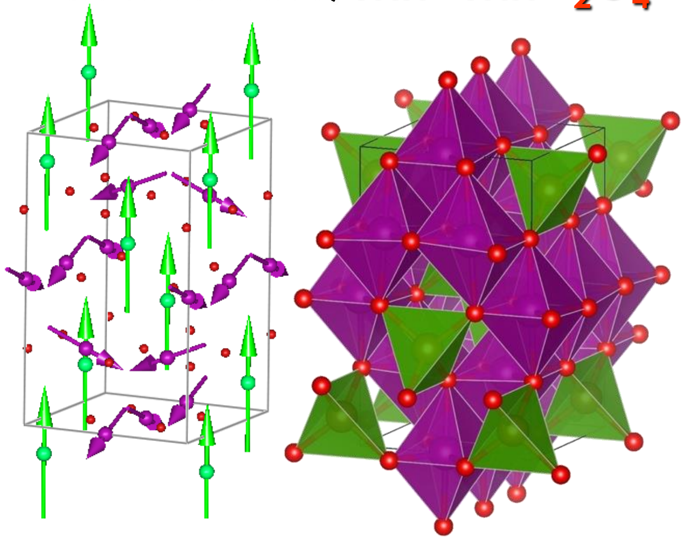
Lectures and hands-on tutorial sessions will cover:

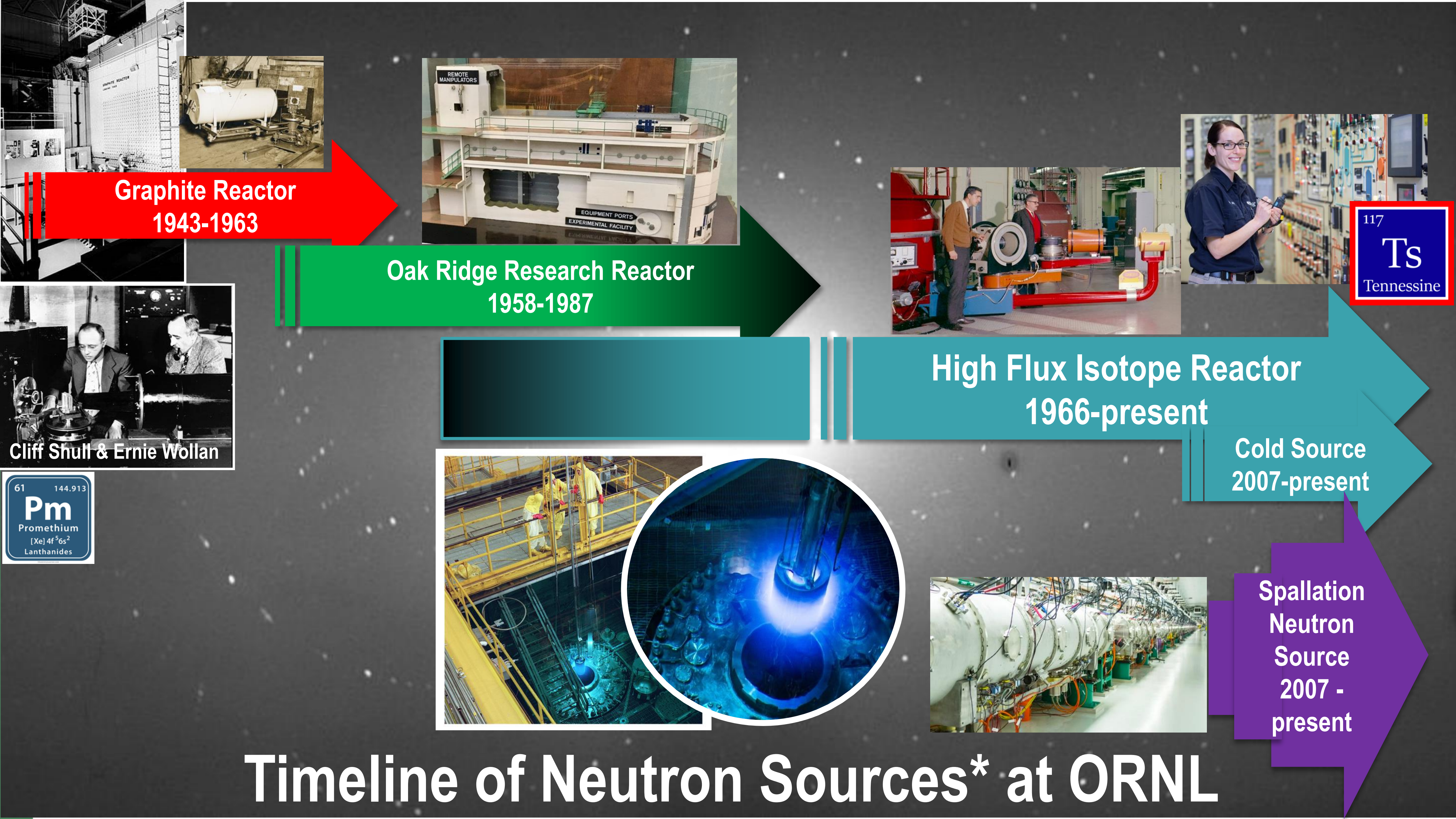
1. Symmetry analysis using representation theory and the SARAh program
2. Magnetic space groups using the Bilbao Crystallographic Server
3. Refinement strategies using the FullProf Suite
4. Magnetic structure determination from powder (constant wavelength and time-of-flight data) and single-crystal data (constant wavelength)

The school is intended for graduate students, postdocs, and research scientists who have a working knowledge of crystallographic refinement and will benefit from incorporating the techniques of magnetic structure determination from neutron diffraction into their research. FullProf software will be used for hands-on examples. (https://www.ill.eu/sites/fullprof/)

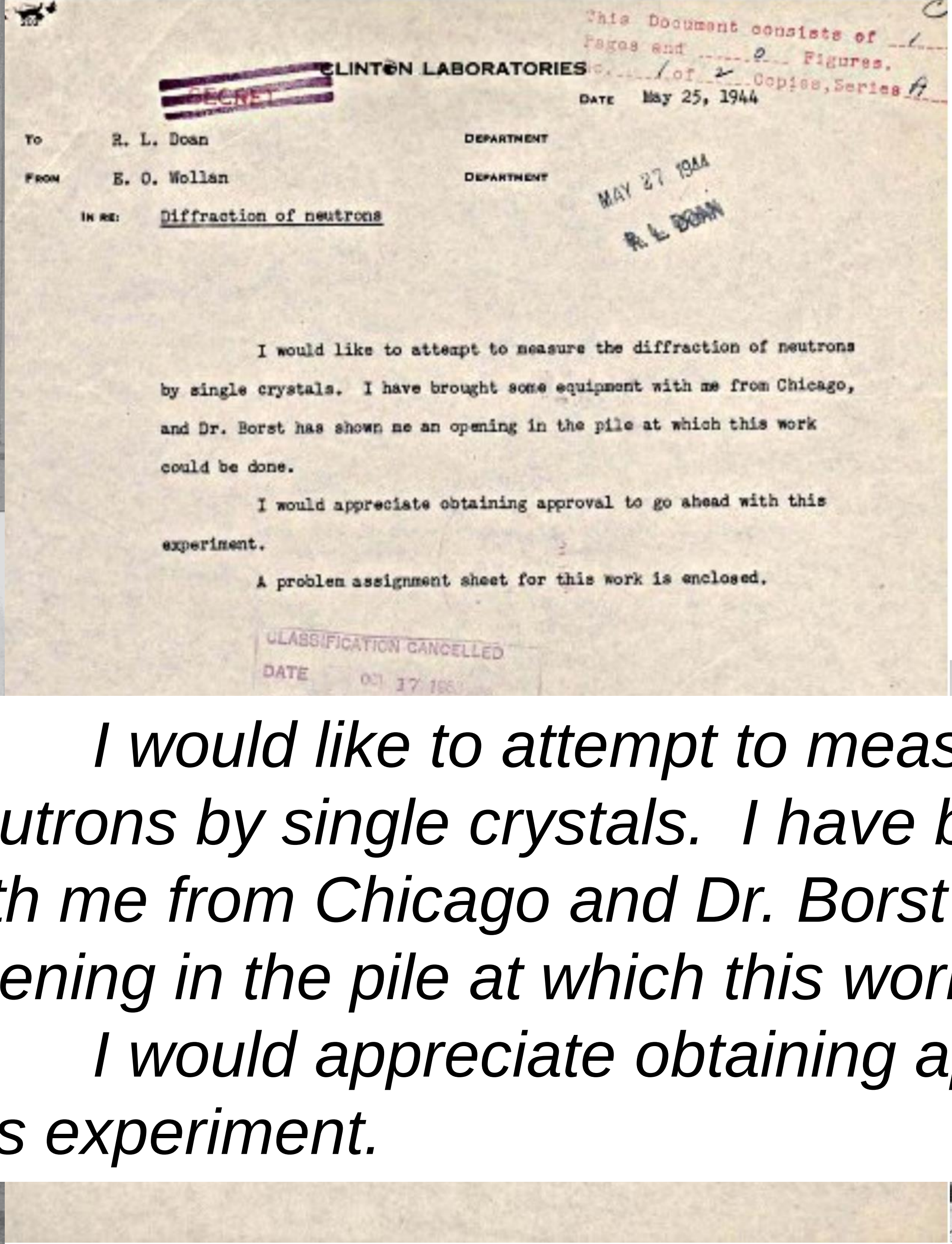


Hausmannite, $Mn^{2+}Mn^{3+}{}_2O_4$





Graphite Reactor
1943-1963
REMOTE MANIPULATORS
EQUIPMENT PORTS
EXPERIMENTAL FACILITY
Oak Ridge Research Reactor
1958-1987
High Flux Isotope Reactor
1966-present
117
Ts
Tennessine
Cold Source
2007-present
Cliff Shull & Ernie Wollan
61
144.913
Pm
Promethium
[Xe] 4f⁵6s²
Lanthanides
Spallation
Neutron
Source
2007 -
present
Timeline of Neutron Sources* at ORNL



This Document consists of 1
Pages and 0 Figures.
No. 1 of 2 Copies, Series

SECRET

CLINTON LABORATORIES

DATE May 25, 1944

TO R. L. Doan DEPARTMENT

FROM E. O. Wollan DEPARTMENT

MAY 27 1944
R. L. DOAN

IN RE: Diffraction of neutrons

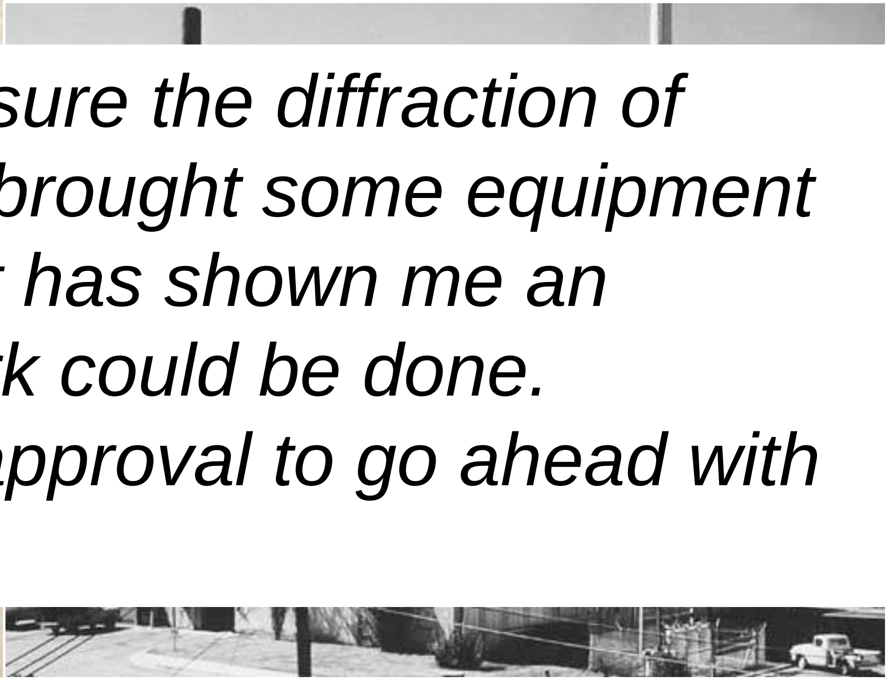
I would like to attempt to measure the diffraction of neutrons by single crystals. I have brought some equipment with me from Chicago, and Dr. Borst has shown me an opening in the pile at which this work could be done.

I would appreciate obtaining approval to go ahead with this experiment.

A problem assignment sheet for this work is enclosed.

CLASSIFICATION CANCELLED
DATE OCT 17 19

The original letter Ernest Wollan wrote in May 25, 1944 to Richard Doan, Director of Research at Clinton Laboratories, requesting approval to do neutron experiments at the X-10 pile.



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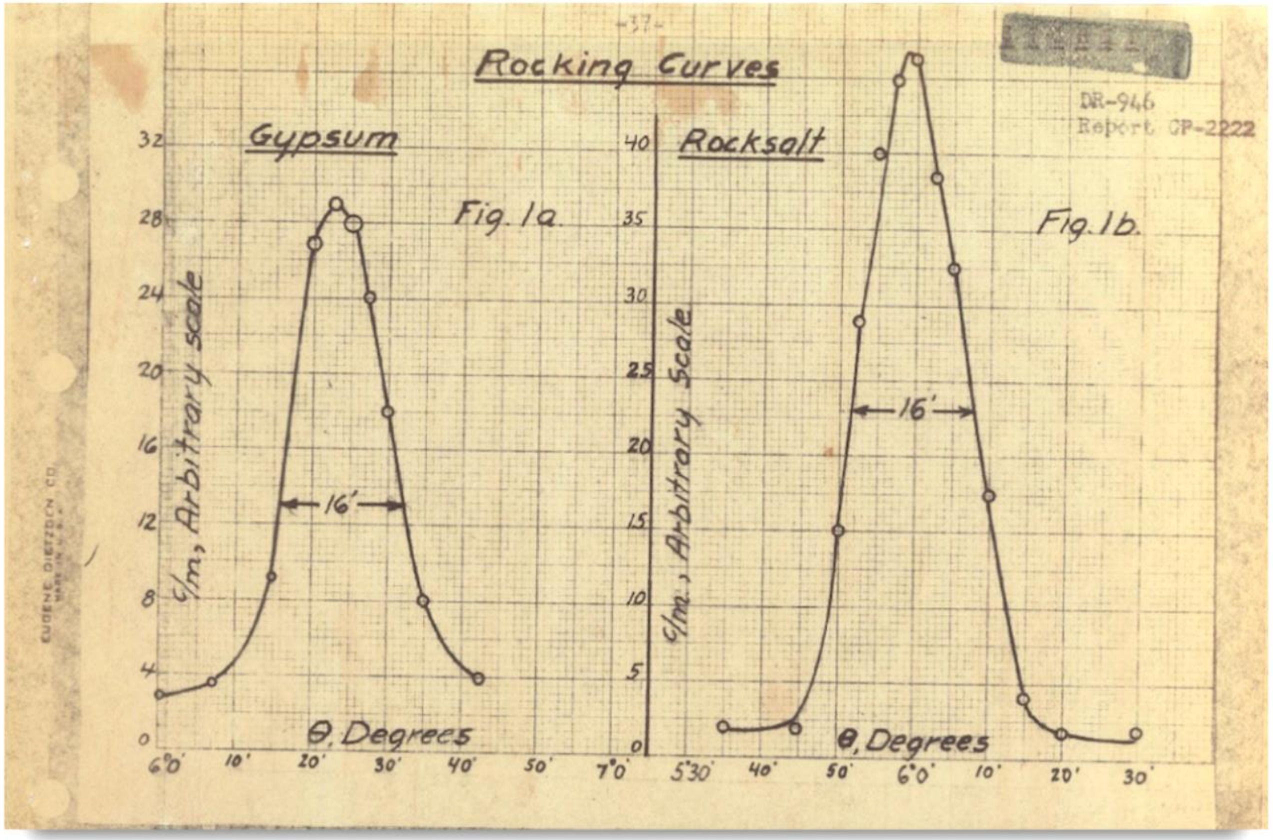
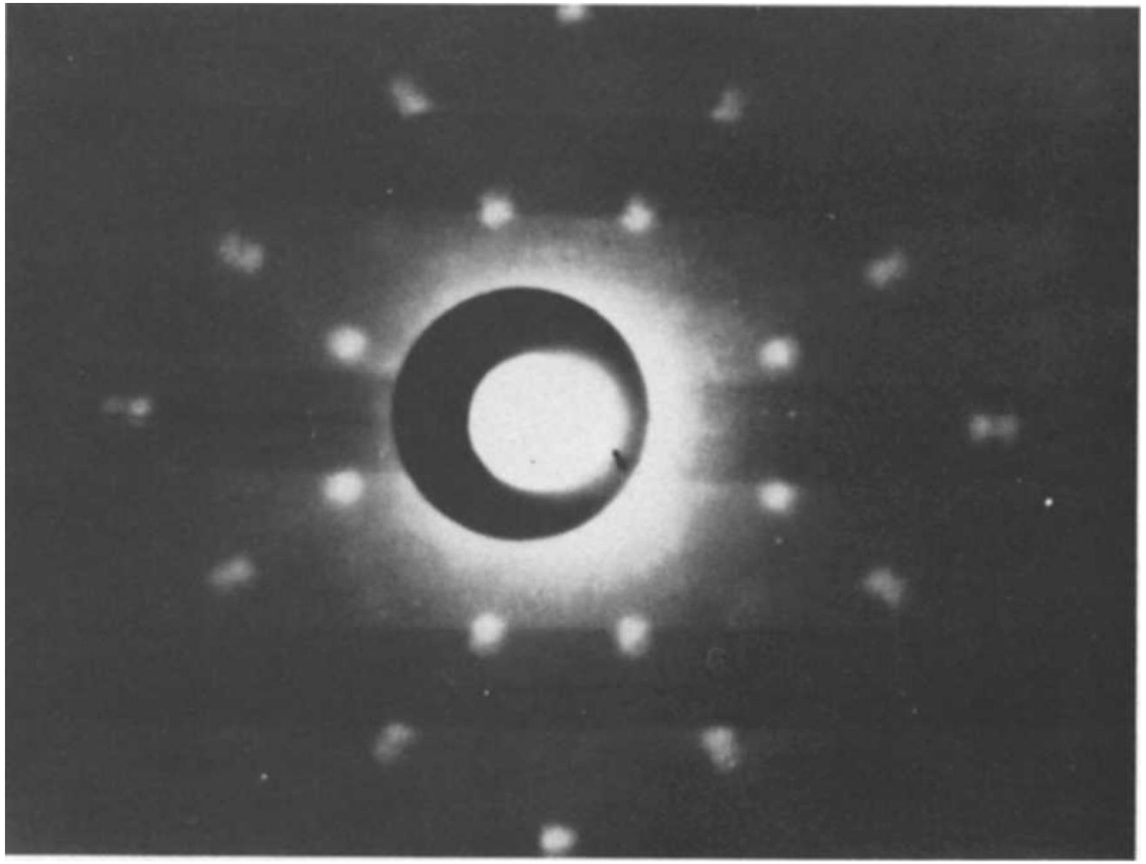




Observation of Bragg reflections via neutron diffraction by Wollan in December 1944 at the Graphite Reactor.

The first neutron Laue diffraction pattern of NaCl measured by Wollan, Shull, and Marney in 1947 at the Graphite Reactor.

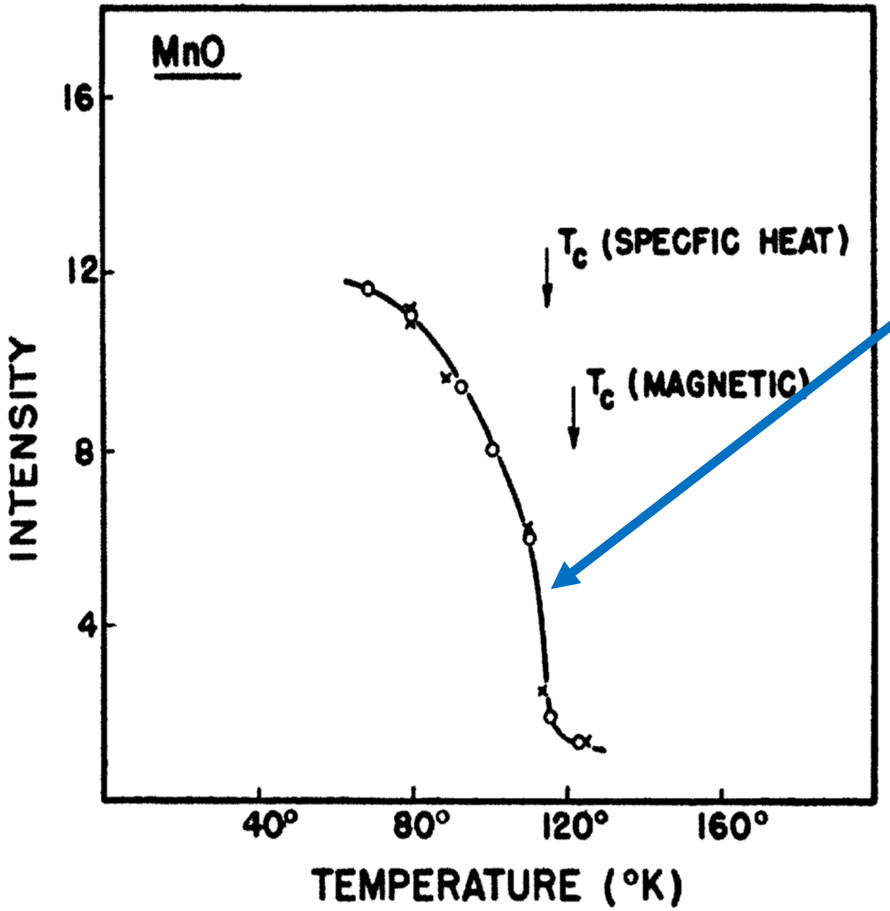
PHYSICAL REVIEW VOLUME 83, NUMBER 2 JULY 15, 1951

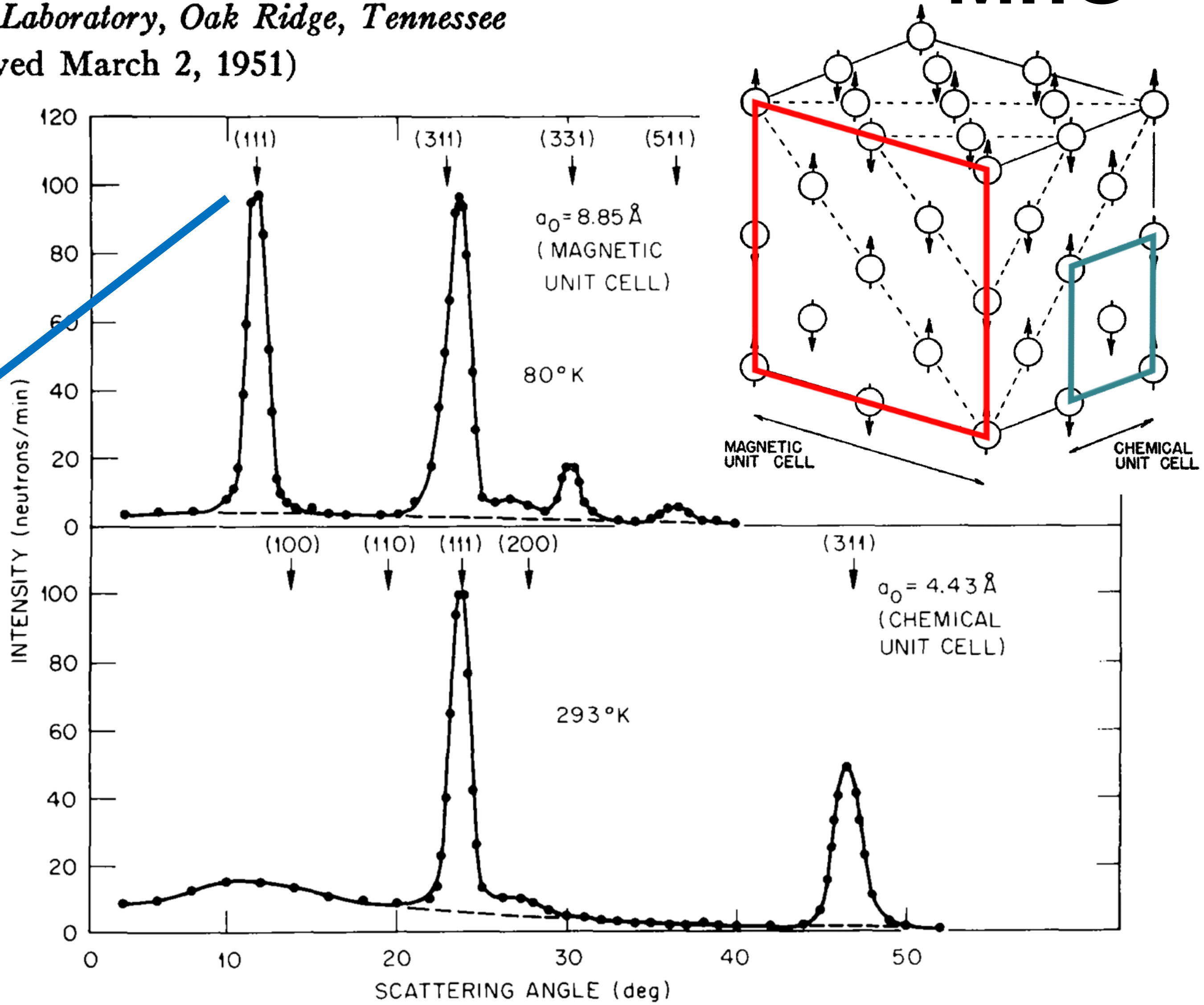
Neutron Diffraction by Paramagnetic and Antiferromagnetic Substances

C. G. Shull, W. A. Strauser, and E. O. Wollan
Oak Ridge National Laboratory, Oak Ridge, Tennessee

(Received March 2, 1951)

MnO





PHYSICAL REVIEW VOLUME 100, NUMBER 2 OCTOBER 15, 1955

Neutron Diffraction Study of the Magnetic Properties of the Series of Perovskite-Type Compounds $[(1-x)La, xCa]MnO_3$†

E. O. WOLLAN AND W. C. KOEHLER
Oak Ridge National Laboratory, Oak Ridge, Tennessee

(Received May 9, 1955)

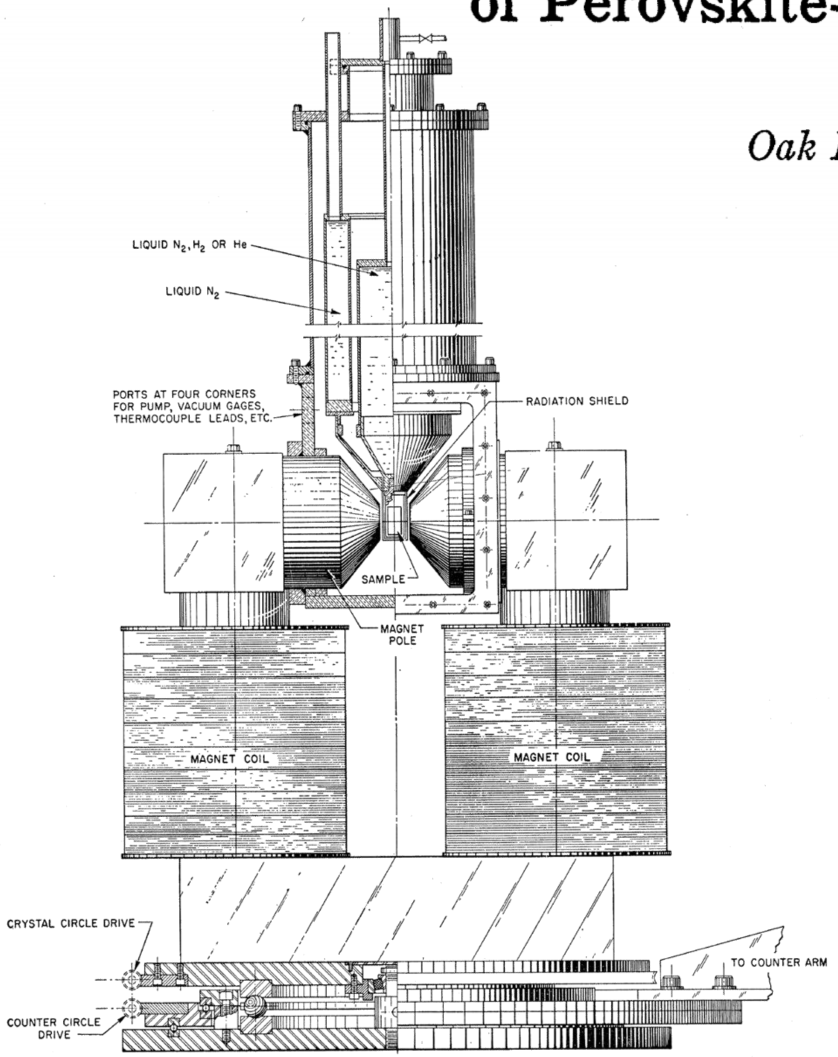
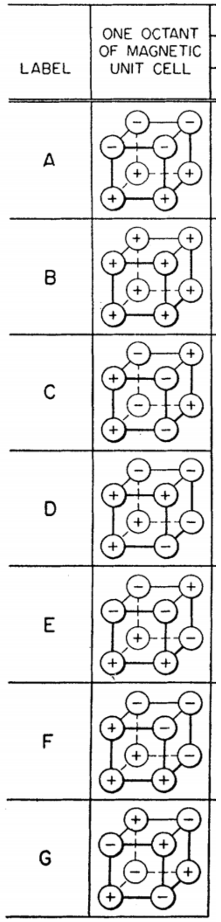
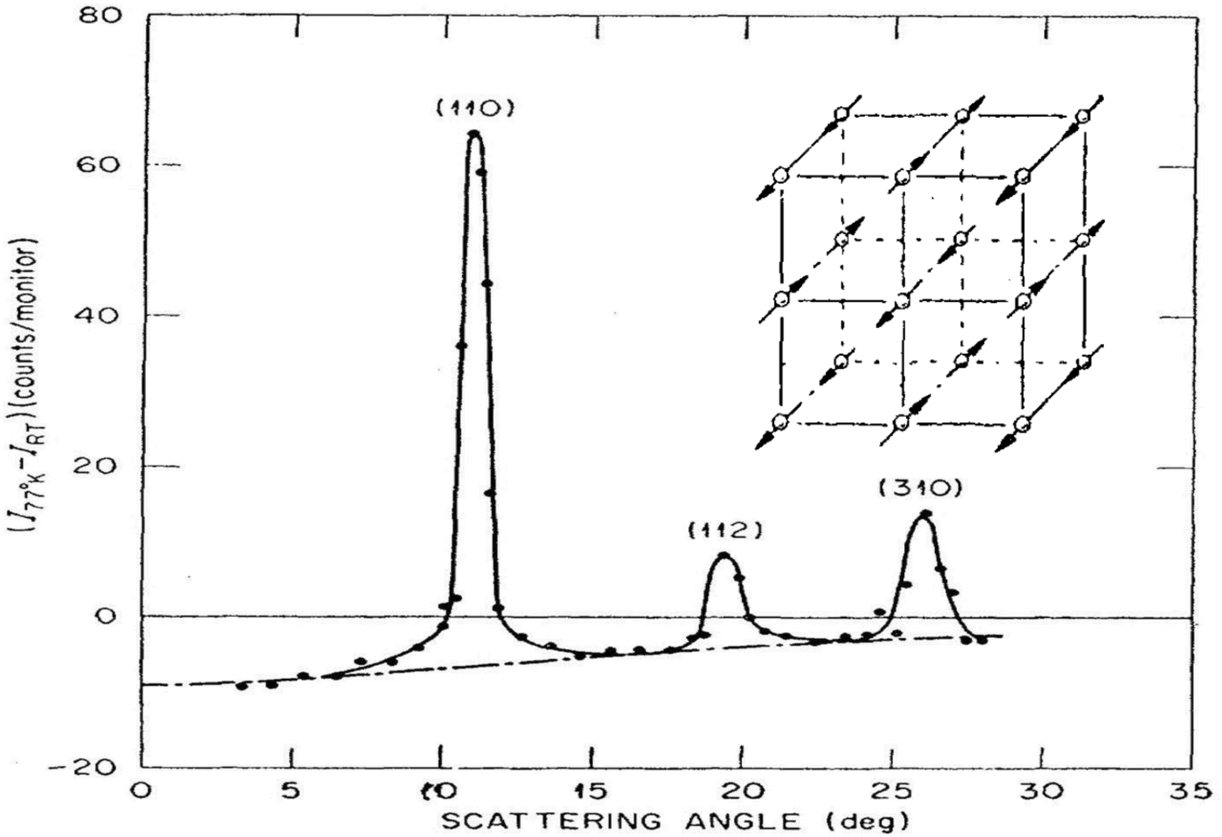


FIG. 1. Neutron spectrometer with cryostat and magnet.





Clifford Shull – selected honors and awards received

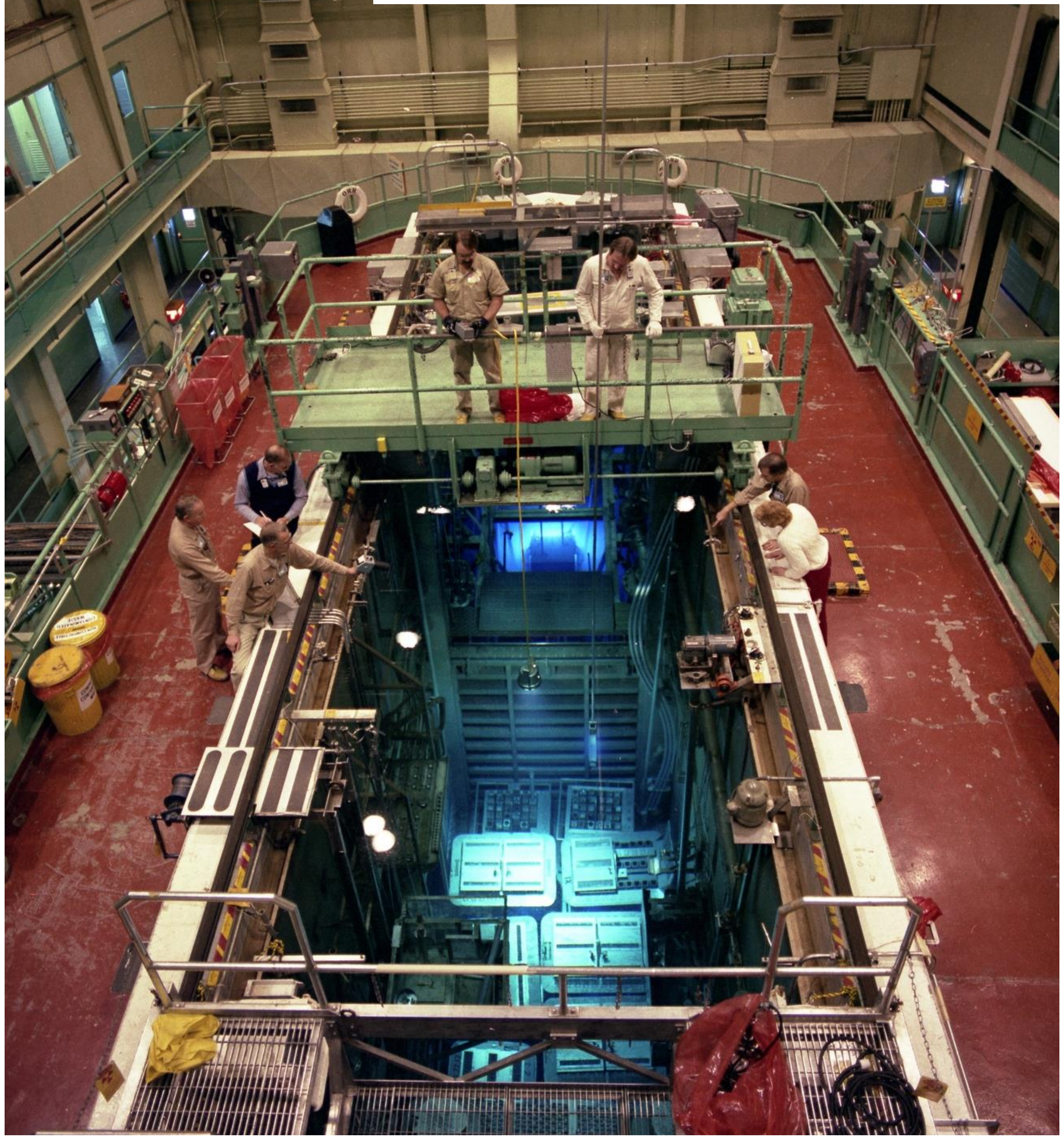
Nobel Prize in Physics, 1994
Gregori Aminoff Prize, 1993
Elected to the National Academy of Sciences, 1975
Oliver E. Buckley Condensed Matter Physics Prize, 1956

For the development and application of neutron diffraction methods for studies of atomic and magnetic structures of solids

1958-1987
20 MW

ORR visitors 1959

ORR Reactor Pool

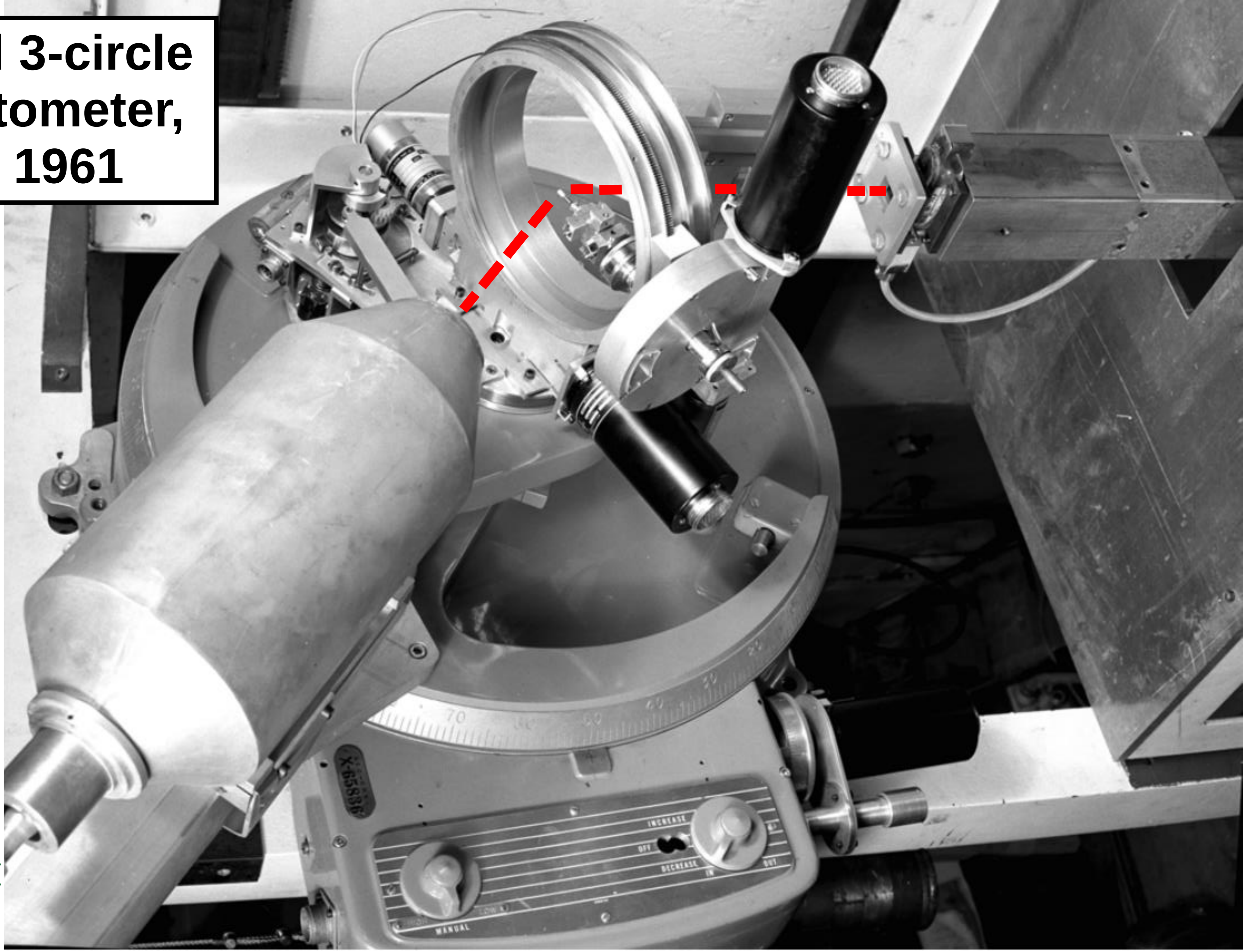


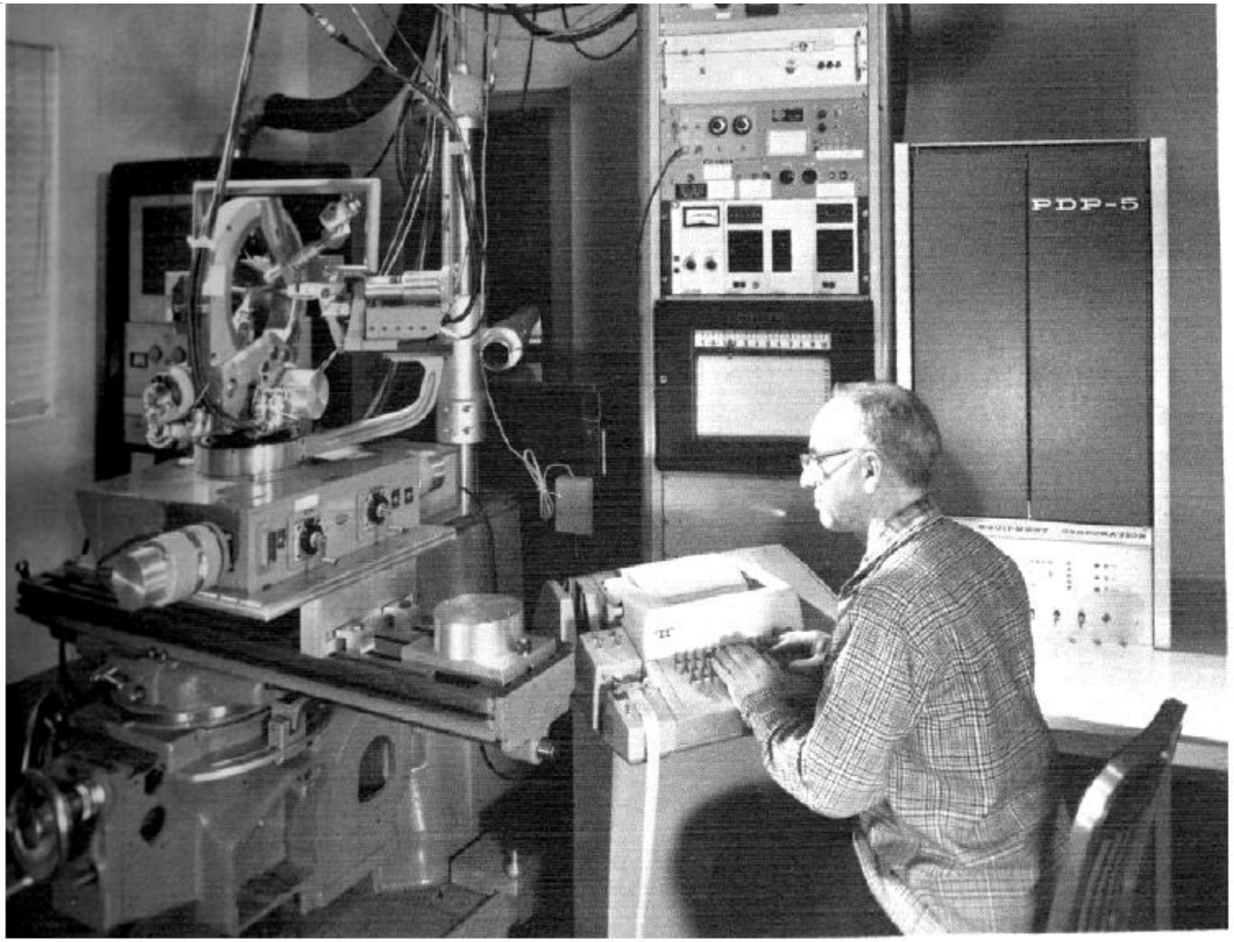
First automated 3-circle neutron diffractometer, ORR in June 1961

ORACLE ("Oak Ridge Automatic Computer and Logical Engine") was used to prepare angle settings which were punched to paper tape

Busing, W.R., H.G. Smith, S.W. Peterson, H.A. Levy, Experience with the Oak Ridge automatic three-circle neutron diffractometer. *Le Journal de Physique* 25, 495-496 (1964).

See Busing memoir https://history.amercrystalassn.org/h-busing_memoir





J.A. Burkhalter
R.B. Splittgerber

Bill Busing
Sharron King

Henri Levy

Development of computer automated X-ray and Four-circle diffractometers at ORNL in mid-1960's

Mathematical recipes and computer programs for crystallography from ORNL

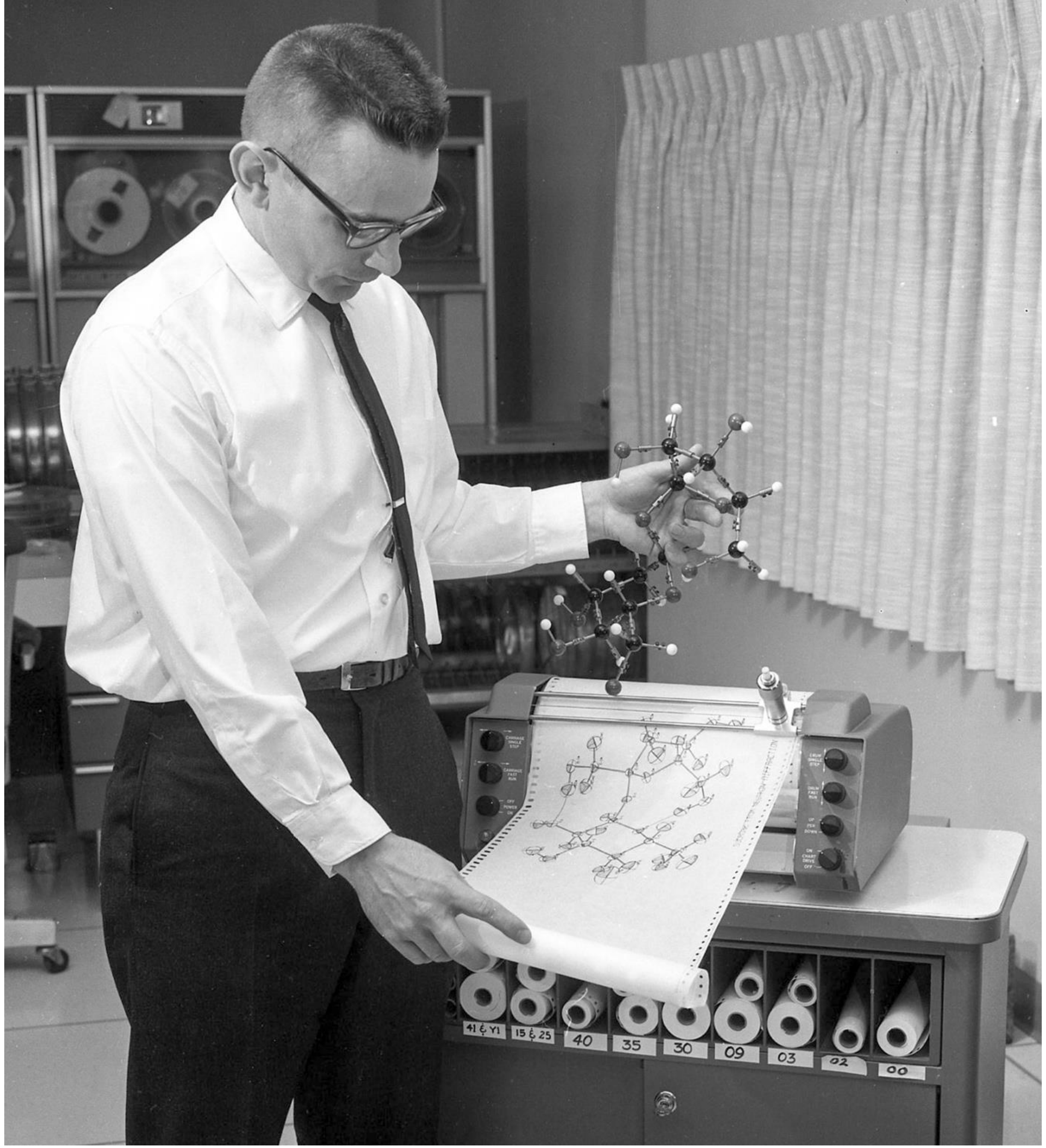
1957 One of the first programs for calculating analytical absorption corrections for single-crystal diffraction studies. Busing, W.R. and Levy, H.A., "High-speed computation of the absorption correction for single crystal diffraction measurements." *Acta Crystallographica* 10, 180-182 (1957).

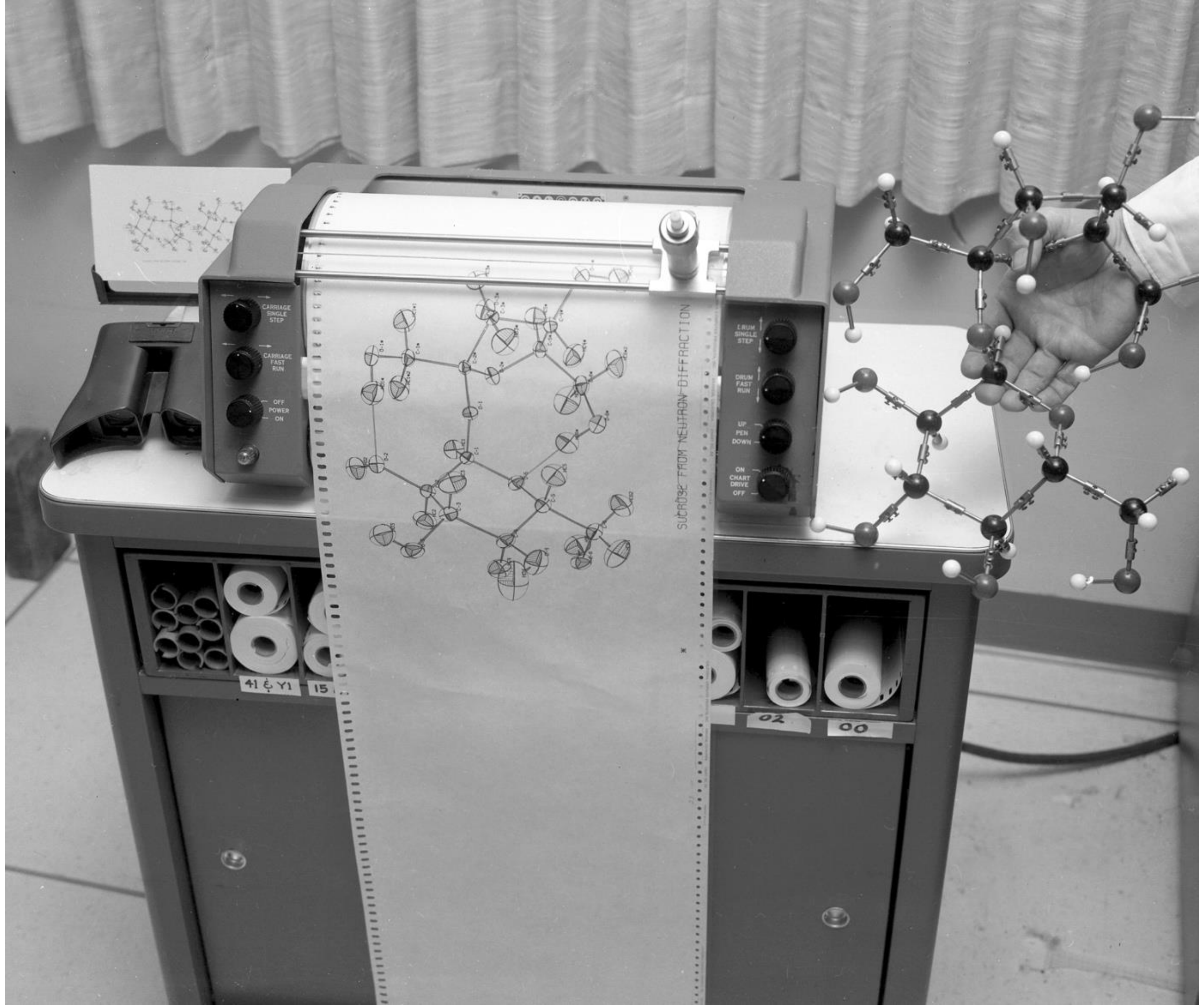
1962 One of the first programs for the least-squares refinement of crystal structures.
Busing, W.R., Martin, K.O., and Levy, H.A., "ORFLS, a Fortran crystallographic least-squares program." Report ORNL-TM-305. Oak Ridge National Laboratory, Oak Ridge, Tennessee.

1964 Bond length corrections for thermal motion
Busing, W.R. and Levy, H.A., "Effect of thermal motion on estimation of bond lengths from diffraction measurements." *Acta Crystallographica* 17, 142- (1964)

1965 Program for plotting atomic displacement parameters
ORTEP, Oak Ridge Thermal Ellipsoid Program. C.K. Johnson, "OR TEP: A FORTRAN thermal ellipsoid plot program for crystal structure illustrations." ORNL-3794 (June, 1965).

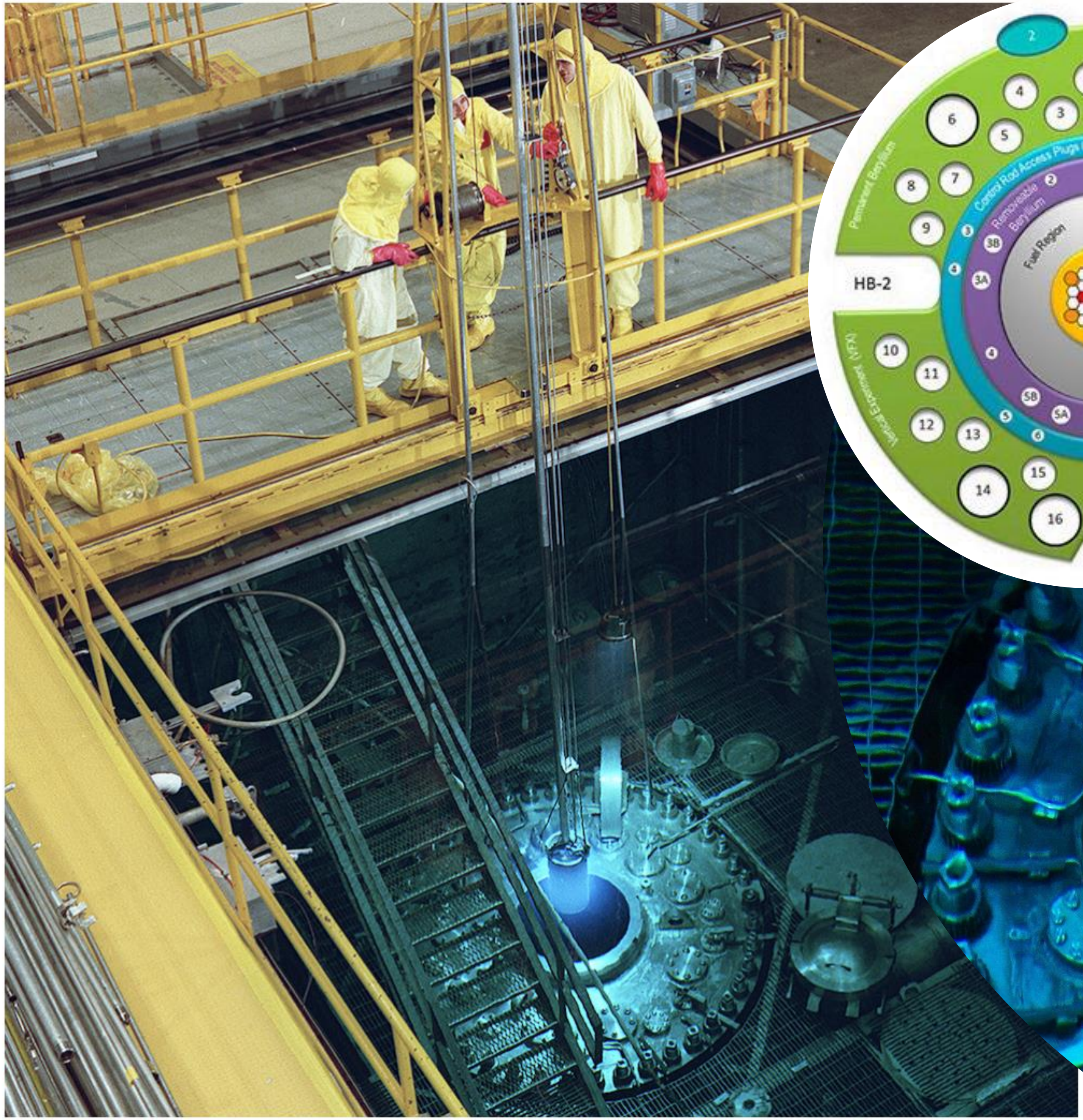
1967 UB Orientation Matrix for single-crystal diffractometry.
Busing, W.R. and Levy, H.A., "Angle calculations for 3- and 4-circle x-ray and neutron diffractometers." *Acta Crystallographica* 22, 457-464 (1967).

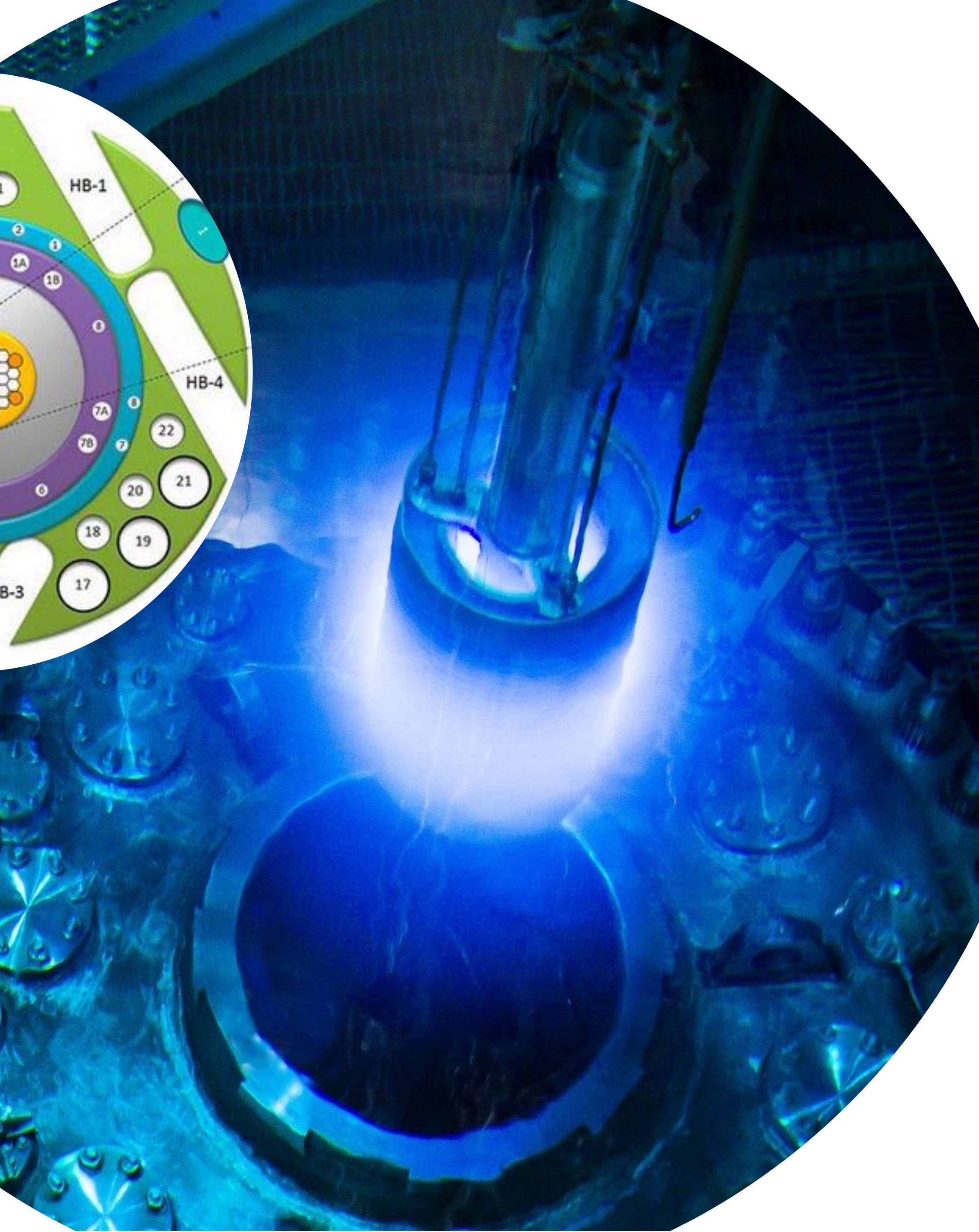


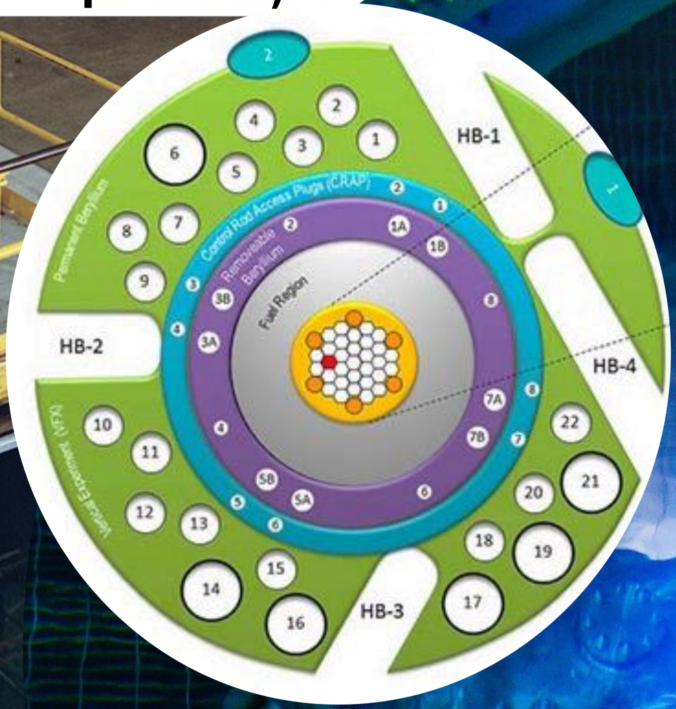


Carroll K. Johnson, “OR TEP: A FORTRAN thermal ellipsoid plot program for crystal structure illustrations.” ORNL-3794 (June, 1965).

HIGH FLUX ISOTOPE REACTOR (1965 – present)







PHYSICAL REVIEW VOLUME 181, NUMBER 2 10 MAY 1969

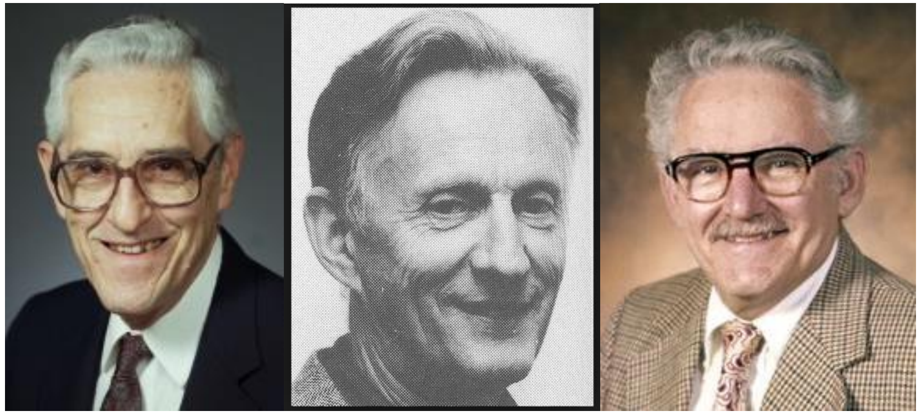
Polarization Analysis of Thermal-Neutron Scattering*

R. M. Moon, T. Riste,† and W. C. Koehler
Solid State Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830

(Received 30 December 1968)

A triple-axis neutron spectrometer with polarization-sensitive crystals on both the first and third axes is described. The calculation of polarized-neutron scattering cross sections is presented in a form particularly suited to apply to this instrument. Experimental results on nuclear incoherent scattering, paramagnetic scattering, Bragg scattering, and spin-wave scattering are presented to illustrate the possible applications of neutron-polarization analysis.

"This technique permits the accurate separation of magnetic scattering from nuclear scattering, and it is used in neutron centers worldwide to study many classes of materials."



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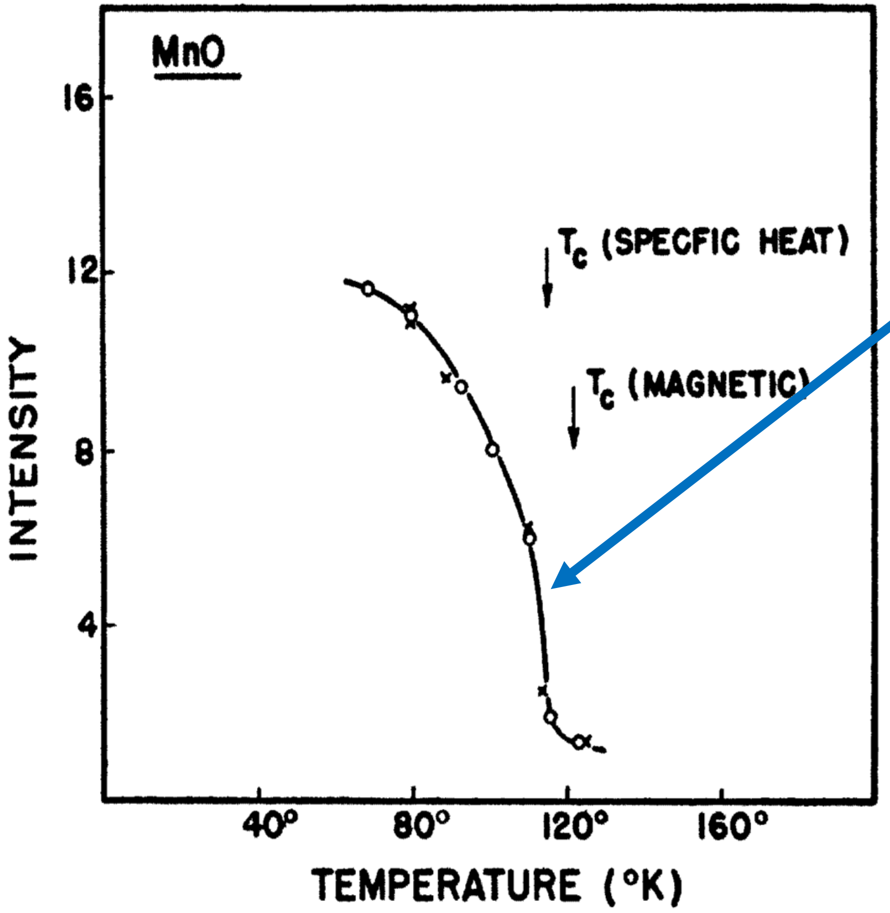
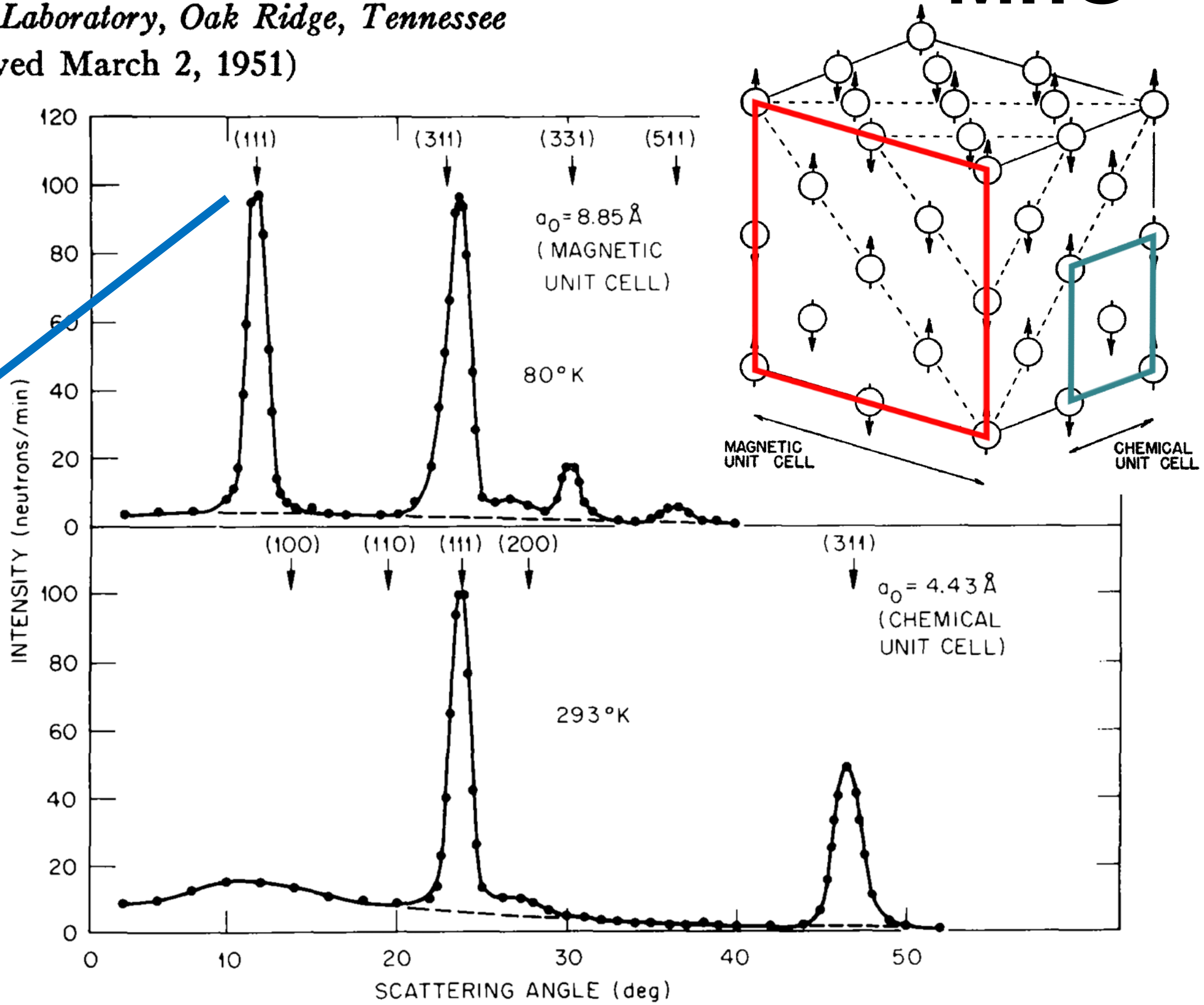




Maximal magnetic space groups for the parent space group *Fm-3m* (No. 225) and the propagation vector k = (1/2, 1/2, 1/2)

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

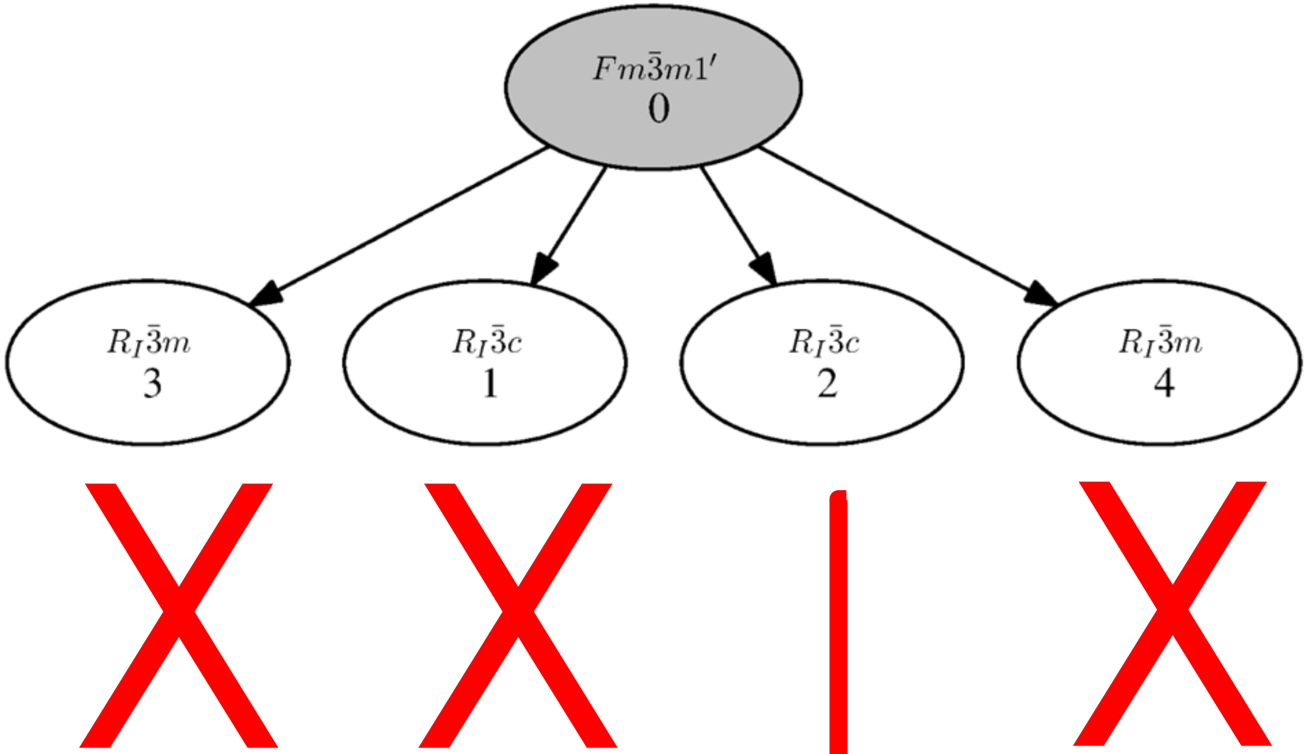
N	Group (BNS)	Transformation matrix	General positions	Properties	Magnetic structure
1	R_I-3c (#167.108) Go to a subgroup	$\begin{pmatrix} 1/2 & 0 & 2 & 0 \\ -1/2 & 1/2 & 2 & 1/2 \\ 0 & -1/2 & 2 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
2	R_I-3c (#167.108) Go to a subgroup	$\begin{pmatrix} 1/2 & 0 & 2 & 0 \\ -1/2 & 1/2 & 2 & 0 \\ 0 & -1/2 & 2 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
3	R_I-3m (#166.102) Go to a subgroup	$\begin{pmatrix} 1/2 & 0 & 2 & 0 \\ -1/2 & 1/2 & 2 & 0 \\ 0 & -1/2 & 2 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show
4	R_I-3m (#166.102) Go to a subgroup	$\begin{pmatrix} 1/2 & 0 & 2 & 0 \\ -1/2 & 1/2 & 2 & 1/2 \\ 0 & -1/2 & 2 & 0 \end{pmatrix}$ Alternatives (domain-related)	Show	*Systematic absences* MAGNEXT *Tensor properties* MTENSOR	Show

Input data

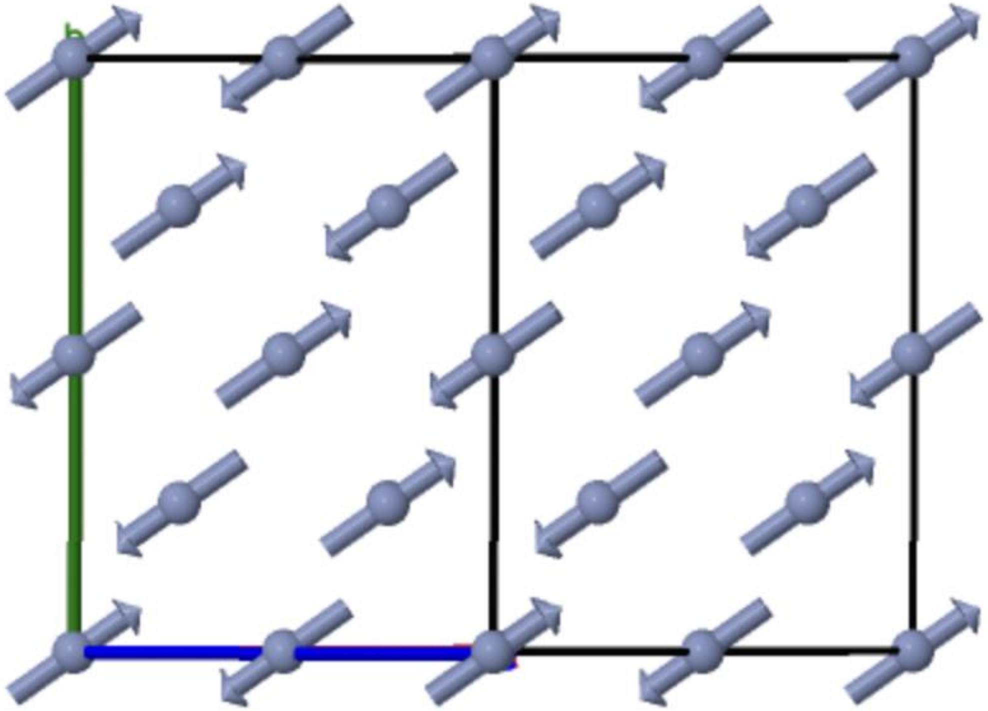
Subgroups of the paramagnetic space group :	$Fm\bar{3}m1'$ (N. 225)
Only maximal subgroups should be shown	
Magnetic propagation wave-vectors	(0.5,0.5,0.5)

Graph of subgroups that fulfill the given conditions

Get the full list of subgroups

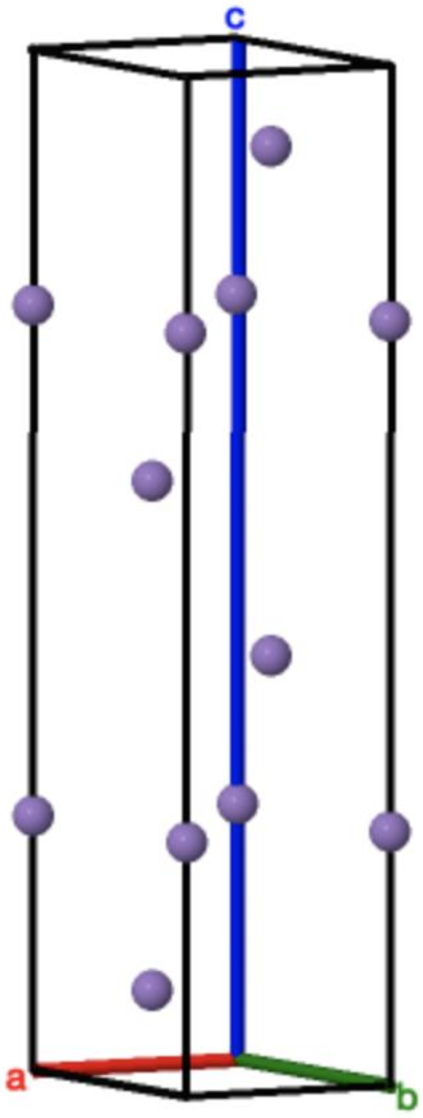


(110) projection

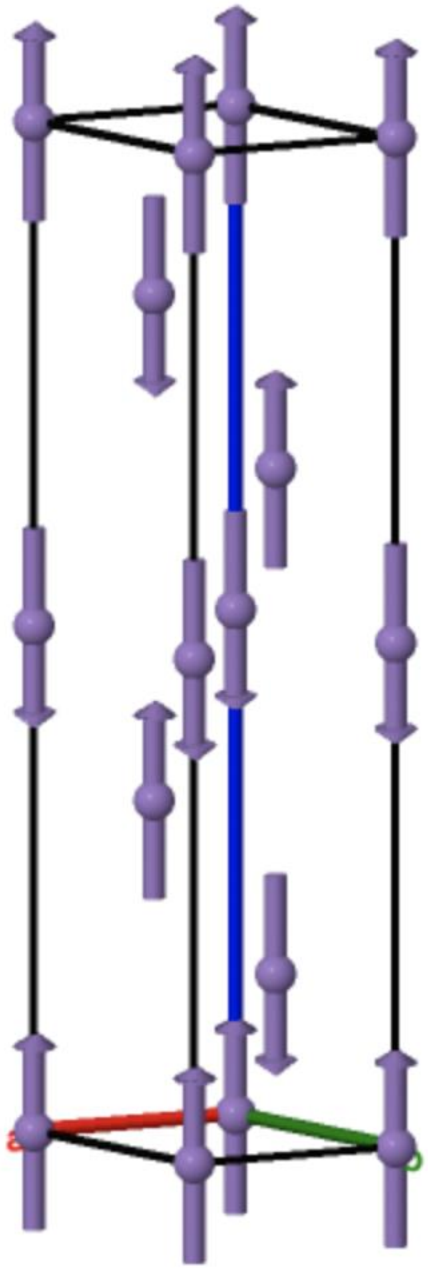


2- $R_I\bar{3}c$ (#167.108)

(M_x,M_x,M_x)



$R_I\bar{3}c$
1



$R_I\bar{3}c$
2