PRNC078

PRNC=78.

PUERTO RICO NUCLEAR CENTER

FORTRAN PROGRAM FOR CALCULATION OF

NEUTRON DIFFRACTION MAGNETIC INTENSITIES

?OPERATED BY UNWERSITY OF PUERTO RICO UNDER CONTRACT

NO. AT (40-1)-1839:FOR U. 5. ATOMIC ENERGY COMMISSION

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PRNC Report

Fortran Progras for Calculation of

Neutron Diffraction Magnetic Intensities

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and

Don T. Cromer

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Introduction

This report presents a fortran progran for
computing the intensities of neutron diffraction
magnetic reflections, It has been written for
the IBH 1620 computer located at the University
of Puerto Rico, Mayaguez, Puerto Rico.
Consequently, all of the input-output is in the
form of READ and PRINT or PUNCH statements.
These statements are duplicated with sinilar

tape stat:

ents preceded by Ct punched in cols.
and 2, Another user might want to remove the
READ, PUNCH and PRINT statements and replace

them with the tape statenents after deleting the

ct,

Another user might alse want to use the
wajor portion of this program as a subroutine

and write a main program which would systen-

atically generate indices and/or spin vectors.

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The Intensity Tunction

the program computes [FC [? = FCW? x rC®

2) = Ep Kk exp(nil @

374

where + DA + tet, @

the reciprocal lattice vector,

potxatybezg, @

ne!

the position vector of the jth atom in the unit cell,

x = was wip ow

yp

a normalized unit vector parallel to the magnetic moment of the

jth atom,

i)

where y is the magnetic moment of the neutron, S is the spin quantum

number of the atom, £ is the orbital form factor, B is the isotropic

temperature factor and e, m, and c are the usual physical constant

eta = e(hat + kbA + toh, 6)

the unit scattering vector and ¢ is the interplaner specing.

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tet

exp(2viltr) = A + iB m

5 3G

where

A= cos 2uiltr = cos 2n(hx + ky + tz)

i GGG

and 8 = sin 2e(hx + ky ¢ tz Dy

G3 4

Then

Fa Kev) = tp KA @

? 3a4 aa

e 2H) = evCertp KA oeCertD KA

Ps3 i935

+ (peas Cp ead

go33 i

= 2(ertp KA) + Cp KAD. @

j735 35

In terns of hy k, t, the cell constants a, by cy a, f y and

components of the normalized spin vectors, my, Mg and my

quation (9) becones

2 2 Bela ety)?

a) = = a? op a Come + emi gt 2

alk Ge Amy tm tty)

ao)

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A similar expression for F,°(H) is obtained by substituting 8 for

A in equation (10),

Then

IPap} = Fan + 7,200 ay

which is the desired result.

Spin vectors read into the machine do not have to be normalized.

The direction of the spin vectors is specified by reading in components

Nye My My which define a vector M with respect to the unit cell axes.

Then for the spin direction of the jth atom,

ar

and

as)

where

Im} = Candy? + Condy? + Condy?

7 1 2

+ 20nd) + Wrdec + Wwrccoee?

2iWiubadcosy + Hiujaccos ¢+ ¥3NIpecoea) as

---Page Break---

Input

card 1 Title information, 72 Hollerith characters.

Card 2 Cell constants aybycyas fay OF @sdscycotay

cost, cosy. Fornat (sF 10:5)

card 3 umber of chemical species (up to 6), number

of each species and number of unpaired electrons

in the species*, Fornat (15, 6(12, F 8.5))

Cards ¥ One form factor card for each species giving 14

values of F at intervals of sin @/A#0.05 starting

at sin 0/20, Linear interpolation fe made.

Format (1uF 5.4)

cards 5 one card for

ach atom (maximum of 84) giving

Xs¥s258 and spin vector components My, Hoy My

parallel to aybycv

Cees We mas Moy + ye) Format (7F 10,5)

Cards 6 One card giving h,k,t for each desired plane

Format (3F 540)

Program ends when blank caré (H = 0) is read.

Press start to read complete nev set of cards,

If sense switch 2 is on, program reads new

data without paus

?Por partially ordered spins, a fractional number of

unpaired electrons can be used.

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Example

Table 1 liste e sample input and Table 2 the

output for the calculation of a few of the magnetic

reflection intensities for FeySid,, There are two

different sets of Four magnetic re?? ions, each set

having a different number of unpaired electrons,

Two forn factor curves must be read in because the

fora factor curve is modified according to the

number of unpaired electrons before it is used.

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Glossary

XNANE Problem identification

a a axis

p > axis

c © axis

ca © or cos a

ce for coe &

ce yor coe y

sa sine

sp sin ¢

sc siny

CASTAR cos at

cBSTAR cos

cOsTAR cos y*

SASTAR sin at

SBSTAR sin ?*

sesTar sin yt

ASTAR an

ESTAR be

csTAR ct

Pr 2

ase a

Bso »?

cso 2

AB abooe ¥

ac acces F

Bc becos a

---Page Break---

NK

wr(x)

SPIN(I)

FoRM(T,J)

134K

omae

xe), 1), 20)

1)

m1), 202), 132)

oo

v1), Y201), ¥3C2)

Hi, 2, HS

◦

psq

sth

SH, NS, TH, SF

ARG

a

BL

SIA, S1B

S2A,. 620

Fs0

wna, wH2, ms

Number of magnetic species

Number of atons of species I in

the cell

Wunber of unpaired electrons in

species I.

The value of the jth point in the

form factor of atom of species I.

Value stored as f aSPIN(1)40.538/2.0.

index variables

Number of atoms in the unit cell

Atom coordinates, unit cell fractions

Temperature factors

Spin vector components Myy Moy My

Magnitude of spin vector

Normalized spin vector components

mye Pay By

bee

aya?

2

sin o/h

Quantities involved in form factor

interpolation

Form factor for reflection hk t

Also used as a temporary variable

in the sunmation of equation (10)

in the 300 0 loop.

E exp (-B sin?e/2?) see equation (5)

2y (nx thy tte)

P eos (ARG)

P sin (ARG)

The first summation in equation (10

The second summation in equation (10)

22 2

Ira [=r 2aperg2cH)

hk £ in integer form

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FE(2)S1O(4) MAGNETIC INTENSITIES

_OELL. CONSTANTS

1. .976 7310 814 .701

4.822

Be

+585

1. 1976 2910 7814 2701 1585

wrororor Nomsunag

x

+987

1012

2487

1512

0000

0:000

+500

1500

aaso-cox

0:

0.

L

1

◦

◦

1

1

◦

1

You

279.250

2720. 1750

1220. 1750

°773 250

1000 0.000

7000 500

£500 0.000

+500 500

F sgo

2.8794

66.8008

121321

B

0.000

02000

9:000

0:00

0.000

97000

0.000

0.000

Teble 2

10.480

COS ALPHA 0.00000 COS ETA 0100000 COS GAMMA 0.60000

THERE ARE 2 ATOMS IN THE CELL

4) WITH 4.95800 UNPAIRED ELECTRONS

4 WITH 3.96200 UNPAIRED ELECTRONS

*W76 6376 .295 .227 173.132 103

2476 376 1295 (227 1173 1132 103

SPIN VECTORS

9.000

92000

0000

0.000

1881

~1881

1881

~1881

0,000 1.000

02000 1.000

92000-1 :000,

02000-1 :000

1230 1.430

£230 1.430

=1230-1.430

1230-1430

ca 6.088

-084

1084

NORMALIZED SPIN VECTORS

?0.0000 0,000

920000 0.0000

070000 0:0000

0.0000 0.0000

10882 10230

(0882 -'0230

10882 -:0230

10882 0230

1642

11642

1162

11642

21432

11432

711432

=11432

---Page Break---

rs

ot

MAGNETIC INTENSITIES

OUTPUT WILL BE PRINTED WITH SENSE SWITCH 1 OFF AND PUNCHED

WITH SENSE SWITCH 1 ON

If SENSE SWITCH 2 15 ON PROGRAM WILL READ NEW DATA SET

WHEN FINISHED. IF SENSE SWITCH 2.18 OFF PROGRAM STOPS,

PRESS. START TO READ WEW DATA SET.

DIMENS 1 ONXHAME (18), NI (6),FORM(6, 14), SPIN(6),X(64),¥(6l),2(64)

TCG) YC) x2 (OHS, X3004) ,¥1 (6h), YB (6H), ¥3LOH) PLEH) ANCOR),

281 (6

1 FORMAT (1845)

2 FORMAT (1H1, 1886)

3 FORMAT (6F10,5)

& FORMAT (15, 6(12,F8.5))

5 FORMAT (14°5,4)

8 rORMAT (7F10.5)

7 FORMAT (314,F10,4)

B FORMAT (25H ii kL F SQUARED)

FORMAT (/72H ATOM XY ZB SPIN VECTORS NORMA.

TLIZEO SPIN VECTORS)

10 FORMAT (14, 76.3, 3X, 37.4)

```
11 FORMAT (/10X, 1HHCELL COWS TANTS/
110K F8.3,11H BeF8.3,12H nF 8.3/,
210HCOS ALF '=F8,5,12H COS GAMMASFS.5/)

12 FORUAT (3

13 FORMAT (i

1 FORMAT (9F

15 FORMAT (7218 HK LF Sg0)

1 FORMAT (13, Sit WITH.F8.5, 19% UNPATRED ELECTRONS)

17 FORMAT ( GfiTHERE ARE,13,13H ATOMS IN THE CELL)

18 FORMAT(F3.0,13°5.3)

READ PROBLEM 1OENTIFI CATION
READ INPUT TAPE 10,1, XWAHE
99 READ 1, XWAME
WRITE QUTPUT TAPE 9,2, XNANE
IF (SENSE SWITCH 1)1600, 1001

1000 PUNCH 1, XNAME
```

GO TO 1002

1001 PRINT 1, XNAME

1002 CONTI NUE

READ CELL CONSTANTS

CELL ANGLES IN DEGREES OR AS COSINES

READ INPUT TAPE 10, 3,A,8,C,CA,CB,CC

READ 3,8,8,C, CA, CB, Cl

SE (CARH .6)404 101, 400

100 CRecosF(cA/57:29578)

j

8)

101 1F(CB=1,0)103,103,1

102 CBacosF(ce/57.29578)

5,1

8

02

103 1F(Co=1.0)105,105, 104

104 comcosF(cC/57.29578)

105 SkmSQRTF(T.0~CA*CA)

SB=SQRTF(120-cB*cB)

SCeSQRTF(120-cc*cc)

CASTAR?(CBRCC~CA)/(SBxSC)

CBSTAR=(CA«CC-cB)/(SA*SC)

CCSTAR=(CAxCB-~CC) /(SAxSB)

---Page Break---

o

1003

100%

1005

1061

1050

1062

1063

1064

om

106s

gooo

1070

1071

1072

109

310

SASTAR=SORTF (1 ,0-CASTAR*CASTAR)

SOSTARGSQRTF (1 LO-CUSTAR*CBSTAR)

SCSTAR=SQRTF (1. 0-CCSTAR*CCSTAR)

ASTARat .0/ (A*SB*SCSTAR)

BSTARa! .0/(B*SA*SCSTAR)

CSTAR=1 10/(C*SA*SESTAR)

WRITE OUTPUT TAPE 9,11,8,0,¢,CA,c8, cc

IF (SENSE SWITCH 1)1003; 1004

PUNCH 11,A,0,C,CA,CB,CE

GO 70 1005)

PRINT 11,4,8,C,CA,CB,CC

CONTI NUE

Pim? .0*3, 141 5926

ACaAsC%CB

BCaBH CCA

READ NUMBER OF SPECIES, NUMBER OF EACH SPECIES AND

NUMBER OF UNPAIRED ELECTRONS IN EACH SPECIES

MAXIMUM NUNDER_OF SPECI ES=6

READ INPUT TAPE 10,4, NK, (NI(1)

READ SNK, (NIC) SPIN(HS T=, 65

WRITE OUTBUT TAPE 9,17,Ne

IF(SENSE SWITCH 1)1060, 1061

PRINT 17,1K

60 TO 1062

PUNCH 17, NK

20 1965 int nk

IF(SENSE SWITCH 1)1063,1064

PUNCH 16,NI(1),SPINCI)

Go To 1085

PRINT 16,81(1) ,SPINCI)

WRITE OUTPUT TAPE 9,16,I(1),SPIN(1)

CONTINUE

00 110 Tet nk

READ MAGNETIC FORM FACTOR TABLE, ONE FOR EACH SPECIES, EACH TABLE

HAS 11h VALUES AT INTERVALS OF'0,05 IN STN(THETA)/LAMBDA

STARTING AT SIN(THETA)/LAMBOA=0.0? LINEAR INTERPOLATION 1S MADE,

```
READ INPUT TAPE 10, 5, (FORK(1,J),J=1, 14)

READ_5,(FORM(I J} dei, 14)

HF (SENSE switch $1076, 1071

PUNCH 18, (FORN(I, J), Jet, 14)

G0 To 1072

PRINT 10, (FORM(1,J),Je1,14)

CONTINUE

0 109 Jmt 14,

FORN(T, J}=FORIN(1 ,J)*SPIN(1)/2.0*0.539

CONTINUE

=o)

0120, 1=1,n«

Katt (1)
```

00 115 Met, k

Jessel

SPIN(I), t=1,NK)

---Page Break---

c

ce

READ X,¥,2, TEMPERATURE FACTOR, AND THREE COMPONENTS OF THE SPIN

VECTOR? Iii REAL CRYSTAL SPACE FOR EACH ATOM IN THE UNIT CELL,

READ INPUT TAPE 10, 6, X(3) p¥(J),Z(J) T(J), X1(4), x2(), X3(J)

115 READ 6, x(5), YC), 203), TIS, x15), X20), X30)

120. CONTINUE

© NORMALIZE SPIN VECTORS

SHAK!

```
DO-130 I=} JAX

rete (14) (Bon 1} (e219 (Bex (1) 4c) 044901) 192.0

Hs CCAveT 1) J (B*x2 (1) CCH CART (HY) *(C#XZCT ) CB (BHD (1)

2(6%x3(1) ) ca)

XNeSQRTF (XI)

YUCT )=X1 (1) 7x8

Y2(1 =x (1)/ XN


430 ¥3(1)=X3.(1)7XN


ont


WRITE OUTPUT TAPE 9,9

IF(SENSE SWITCH 1)1006,131


1006 PUNCH 9,


131


GO TO 1007

PRINT 9


1007 CONTINUE


cm
```

00135 fat, JHAX

C2435 WRITE OUTPUT TAPE 9,10,1,X(1),¥(1),201),T(1),X1(1), X201),X3(1),

TLC) ,Y2(1) ,¥3 (1)

LF(SERSE SWITCH 1) 1008, 100

1008 PUNCH 10,1 sXC1) 411), 204 D5 9C1) X14), x2(1) 301), YF (1), ¥2C1),Y3C1)

GO TO 135

1009 PRINT TO,1 XH), ¥C1) 4201), THN) XVCH), X2C1) X3C1), ¥1(1),¥2(1),¥3(1)

©

135 CONTINUE

WRITE OUTPUT TAPE 9,15

IF(SENSE SWITCH 1)1017, 1010

1010 PRINT 15

ton

1012

c

©

GO To 1012

PUNCH 15

?CONTI NUE

READ HKL FOR THE DESIREO REFLECTIONS. PROBLEM ENDS WHEN BLANK

CARD I'S READ.

G*200 READ INPUT TAPE 10,12,H41,H2,H3

200 READ 12,1 ¢H2,H3

201

204

1 (ABSF (111 J »ABSF (#2)sABSF (H3))201 , 500,201

(HT*ASTAR)* (HI ?AS TAR) +(H2 "BS TAR} (H2*BS TAR) + (H3*CSTAR)*(H3*CSTAR

1)42 .0%((Hg-"BSTAR) *(143*CS TAR)*CASTAR+ (HI *ASTAR)*(H3*CSTAR) #CBSTAR+

2.(HTSASTAR)*(H2*BSTAR)*CCSTAR)

B51 2070

FORM FACTOR INTERPOLATION

STLe0. 5/SQRTF (DSQ)

SN=STL/0,05

NS=SW

DO 210 Ia1,uk

Ken 1)

E=FORM(1 ,NS+1)~(FORM(1,NS+1)-FORM(1 ,NS+2))*SF

00 205 Mat, k

---Page Break---

205

210

230

250

300

co

1015

1016

1017

500

501

(I

TOY ECR) Bey (L813 K)#ACHY2 (I

JeJel

P(J)mE*EXPF (~0,25*Q*T())

CONTI NUE

00 230 tm1, JHAX

AnGSPr CTARCL Datpey (I)oi3¥Z(1))

ANC xcOsF (ARG) ¥2(1}

MAX

CYC JH sy2 (1)#H2+¥3(1)4H3)

STASSTASAI (1)*E

$1B=518+81(1) RE

DO 250 Kel, JMAX

Envi (1) *¥1 Ui)*asQey2 (1

(ewosgeyacs yrva(xiscsae

*Y3(K) BC) 2.0

SZA=S2A+E%A (1)*A1 (K

?S2BeS284E%B1 (1)*B1(K)

CONTI NUE

FSQ=-DSQ"(S1A*SIA+S1 B*S18)+S2AsS26

NHT

3

WRITE OUTPUT TAPE 9,7, NHI ,NH2, NHB, FSQ

```
IF(SENSE SWITCH 1)1015, 1016

PUNCH 7, NAT, NH2, NH3,FSQ

GO To 1017

PRENT 7, HT, NH2, NH3,FSQ

CONTI NUE

Go 70 200.

IF(SENSE SWITCH 2)99, 501

PAUSE

GO T0 99

END
```

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