PRNC=78. PUERTO RICO NUCLEAR CENTER FORTRAN PROGRAM FOR CALCULATION OF NEUTRON DIFFRACTION MAGNETIC INTENSITIES ‘OPERATED BY UNIVERSITY OF PUERTO RICO UNDER CONTRACT NO. AT (40-1)-1839: FOR U.S. ATOMIC ENERGY COMMISSION ---Page Break--- PRNC Report Fortran Program for Calculation of Neutron Diffraction Magnetic Intensities Met. Kay and Don T. Cromer ---Page Break--- Introduction This report presents a Fortran program for computing the intensities of neutron diffraction magnetic reflections. It has been written for the IBM 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 similar tape statements preceded by C punched in cols. 1 and 2. Another user might want to remove the READ, PUNCH and PRINT statements and replace them with the tape statements after deleting the C. Another user might also want to use the major portion of this program as a subroutine and write a main program which would systematically generate indices and/or spin vectors. ---Page Break--- The Intensity Function 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 constants eta = e(hat + kbA + toh, 6) the unit scattering vector and ¢ is the interplanar spacing. ---Page Break--- tet exp(2πltr) = A + iB m 5 3G where A= cos 2πltr = 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 terms of hy k, t, the cell constants a, b, c a, f

y and components of the normalized spin vectors, my, Mg and my equation (9) becomes 2 2 Bela ety)? a) = = a? op a Come + emi gt 2 alk Ge Amy tm tty) ao) ---Page Break--- 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. Format (sF 10:5) card 3 number of chemical species (up to 6), number of each species and number of unpaired electrons in the species*, Format (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 is made. Format (1uF 5.4) cards 5 one card for each 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 card (H = 0) is read. Press start to read complete new set of cards. If sense switch 2 is on, program reads new data without pause. For partially ordered spins, a fractional number of unpaired electrons can be used. ---Page Break--- Example Table 1 lists a 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 form factor curves must be read in because the form factor curve is modified according to the number of unpaired electrons before it is used. ---Page

Break--- 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 summation 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 ---Page Break--- ---Page Break--- 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 0.0000 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 NEW DATA SET. DIMENS 1 ONXHAME (18), NI (6), FORM(6, 14), SPIN(6), X(64), ¥(61), 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 FORMAT (7F10.5) 7 FORMAT (314, F10, 4) B FORMAT (25H ii kL F SQUARED) FORMAT (/72H ATOM XYZ 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 FORMAT (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 IDENTIFICATION READ INPUT TAPE 10, 1, XWAHE 99 READ 1, XWAME WRITE OUTPUT TAPE 9, 2, XNANE IF (SENSE SWITCH 1) 1600, 1001 1000 PUNCH 1, XNAME GO TO 1002 1001 PRINT 1, XNAME 1002 CONTINUE 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 CONTINUE 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 ‘CONTINUE READ HKL FOR THE DESIRED REFLECTIONS. PROBLEM ENDS WHEN BLANK CARD IS 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()) CONTINUE 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) CONTINUE 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 PRINT 7, HT, NH2, NH3,FSQ CONTINUE GO 70 200. IF(SENSE SWITCH 2)99, 501 PAUSE GO TO 99 END ---Page Break---