PRASEODYMIUM

```
      GOTO 900
  325 IF(IH.GT.NHS) GOTO 900
      IF(IH.GT.50) GOTO 900
      FIH=FLOAT(IH-1)
CALCULATE APPLIED MAGNETIC FIELD RHA
      RHA=RHL+FIH*RHS
      IF(ID.EQ.0) GOTO 330
C
CONSTPUCT THE HAMILTONIAN MATRICES FOR THE ENERGY OF THE IONS
CONSIDERING THE INTERNAL MAGNETIC FIELD AND THE
CRYSTAL FIELD ENERGY LEVELS. UNITS ARE KELVIN.
C
      HZC=0.0
      HZH=0.0
      HXC=(RHA+PM1*RMAGC+RM2*RMAGH)*CU*0.50
      HXH=(RHA+RM1*RMAGH+RM2*RMAGC)*CU*0.50
      GOTO 340
  330 HXC=0.0
      HXH=0.0
      HZC=(RHA+RM1*RMAGC+RM2*RMAGH)*CU
      HZH=(RHA+RM1*RMAGH+RM2*RMAGC)*CU
  340 CALL PRH(RHH,0,HXH,HZH,BH2,BH4,BH6)
      CALL PRH(RHC,1,HXC,HZC,BC2,BC4,BC6)
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
CALCULATE THE EIGENVALUES AND EIGENVECTORS OF THE TWO MATRICES
C
C       ROUTINES F01AJF+F02AMF ARE STANDARD LIBRARY ROUTINES(NAG)
C       WHICH CALCULATE EIGENVALUES AND EIGENVECTORS OF REAL
C       SYMMETRIC MATRICES BY HOUSEHOLDER REDUCTION TO TRI-
C       DIAGONAL FORM FOLLOWED BY THE QR ALGORITHM TO COMPLETE
C       THE DIAGONALISATION.
C       FOR DETAILS OF HOUSEHOLDER AND QP ALGORITHMS SEE BOOKS ON
C       NUMERICAL METHODS, FOR EXAMPLE ACTON R.S. "NUMERICAL METHODS
C       THAT WORK" PUBLISHED BY HARPER,N.Y. (1970) PAGE 347
C
C
C  THE PARAMETER LIST OF F01AJF(N,TOL,A,IA,D,E,Z,IZ) IS
C       N=INTEGER,THE OPDER OF MATRIX A
C       TOL=REAL,MACHINE DEPENDENT CONSTANT, FOR ICL 1900 TOL=2.0**(-218)
C       A=REAL ARRAY,OF DIMENSION AT LEAST(N,N) CONTAINING THE SYMMETRIC
C             MATRIX,THE LOWER TRIANGLE ONLY IS REQUIRED. THE ARRAY IS
C             NOT OVERWRITTEN BY THE ROUTINE.
C       IA=INTEGER,THE FIRST DIMENSION OF A AS DEFINED IN THE CALLING.
C       D=REAL ARRAY,OF DIMENSION AT LEAST (N), ON EXIT IT CONTAINS THE
C             DIAGONAL ELEMENTS OF TRIDIAGONAL MATRIX.
C       E=REAL ARRAY,OF DIMENSION AT LEAST (N), ON EXIT IT CONTAINS THE
C             N-1 OFF DIAGONAL ELEMENTS OF TPIDIAGONAL MATRIX.
C       Z=REAL ARRAY,OF DIMENSION AT LEAST (N,N). ON EXIT IT CONTAINS
C             THE ORTHOGONAL MATRIX Q THE PRODUCT OF THE HOUSEHOLDEP
C             TRANSFORMATIONS.
C       IZ=INTEGER,THE FIRST DIMENSION OF Z AS DEFINED IN CALLING SEG.
C
C
C  THE PARAMETER LIST OF F02AMF(N,ACC,D,E,Z,IZ,IFAIL) IS
C       N=INTEGER,THE ORDER OF TRIDIAGONAL MATRIX T.
```

PRASEODYMIUM

```
C      ACC=REAL,SMALLEST NUMBER ON THE COMPUTER SUCH THAT 1+ACC=1
C            (ON ICL 1900 ACC=2.0**(-37))
C      D=REAL ARRAY,OF DIMENSION AT LEAST (N),CONTAINING DIAGONAL
C            ELEMENTS OF T.
C      E=REAL ARRAY,OF DIMENSION AT LEAST (N) CONTAINING THE SUB-
C            DIAGONAL ELEMENTS OF T STORED IN E(2)-=E(N). IT IS
C            OVERWRITTEN BY THE ROUTINE.
C      Z=REAL ARRAY, DIMENSION AT LEAST (N,N), IF EIGENVECTORS OF THE
C            FULL SYMMETRIC MATRIX ARE REQUIRED IT SHOULD CONTAIN THE
C            Q (SEE F01AJF). ON EXIT IT CONTAINS THE NORMALIZED
C            EIGENVECTORS SUCH THAT Z(I,J),I=1,N CORRESPONDS TO
C            EIGENVALUE J.
C      IZ=INTEGER,THE FIRST DIMENSION OF Z AS DECLARED.
C      IFAIL=INTEGER FLAG, GOVERNS ON ENTRY THE TYPES OF FAILURE
C            THAT WILL BE DETECTED,ON EXIT THE TYPE OF FAILURE.
C            IFAIL=0 ON EXIT FOR SUCCESSFUL COMPLETION.
C
C**********************************************************************
C
C  NOTE THAT IF NAG LIBRARY ROUTINES ARE NOT AVAILABLE THEN THESE
C      ROUTINES HAVE THEIR EXACT EQUIVALENTS IN MOST SCIENTIFIC
C      LIBRARIES( UNDER DIFFERENT NAMES AND WITH, POSSIBLY, DIFFERENT
C      ARGUMENT LISTS)
C**********************************************************************
C THOSE INTERESTED IN NUMERICAL EIGENVALUE PROBLEMS SHOULD CONSULT
C MARTIN R.S.,REINSCH C.,WILKINSON J.H.,NUM.MATH.BAND(11)181-95(1968)
C  BOWDLER H,MARTIN R.S.,REINSCH C.,WILKINSON J.H,
C                         NUM MATH BAND(11) 293-306 (1968)
C************************************************************************
      IFAIL=0
      CALL F01AJF(9,2.0**(-218),RHH,9,EVALH,USE,PHH,9)
      CALL F02AMF(9,2.0**(-37),EVALH,USE,PHH,9,IFAIL)
      IF(IFAIL.EQ.0) GOTO 345
      WRITE(2,2000)
      IFAIL=0
  345 CONTINUE
      CALL F01AJF(9,2.0**(-218),RHC,9,EVALC,USE,RHC,9)
      CALL F02AMF(9,2.0**(-37),EVALC,USE,RHC,9,IFAIL)
      IF(IFAIL.EQ.0) GOTO 346
      WRITE(2,2000)
      IFAIL=0
  346 CONTINUE
      IF(IP.EQ.0) GOTO 349
      IF(IT.GT.1) GOTO 349
      WRITE(2,2005)
      IF(ID.EQ.0) GOTO 347
      WRITE(2,2006) RHA
      GOTO 348
  347 WRITE(2,2007)RHA
  348 CONTINUE
      WRITE(2,2001)
C
C  PRINT EIGENVALUES AND EIGENVECTORS IF REQUIRED
C
      IE=1
      IV=9
```

PRASEODYMIUM

```
      CALL PRINTM(EVALH,1,9,IE)
      WRITE(2,2002)
      CALL PRINTM(RHH,9,9,IV)
      WRITE(2,2003)
      CALL PRINTM(EVALC,1,9,IE)
      WRITE(2,2002)
      CALL PRINTM(RHC,9,9,IV)
  349 CONTINUE
C
CALCULATE THE MAGNETIZATION ON BOTH SITES
C
      IF(ID.EQ.0) GOTO 350
      CALL PRT(9,RHC,EVALC,T,RXO,USE1)
      CALL PRT(9,RHH,EVALH,T,RXO,USE2)
      GOTO 360
  350 CALL PRT(9,RHC,EVALC,T,RZO,USE1)
      CALL PRT(9,RHH,EVALH,T,RZO,USE2)
  360 USE1=-0.80*USE1
      USE2=-0.80*USE2
C
CHECK FOR CONVERGENCE OF MAGNETIZATION
C
      XX=ABS(USE1-RMAGC)
      YY=ABS(USE2-RMAGH)
      IF(XX.GT.0.20) GOTO 390
      IF(YY.LE.0.20) GOTO 400
  390 RMAGC=USE1
      RMAGH=USE2
      GOTO 320
  400 CONTINUE
C
C STORE RESULTS IN ARRAY RES
C
      RES(IH,1)=T
      RES(IH,2)=RHA
      RES(IH,3)=USE1
      RES(IH,4)=USE2
      RES(IH,5)=0.50*(USE1+USE2)
C
CHECK WHETHER REQUISITE NUMBER OF FIELD STEPS HAVE BEEN
COMPLETED AND IF SO OUTPUT THE RESULTS TO LINEPRINTER
C
      IF(IH.LT.NHS) GOTO 310
  900 CONTINUE
C
CONSTRUCT A TABLE OF RESULTS
C
      WRITE(2,2004)
      WRITE(2,2008)
      CALL PRINTM(RES,50,5,NHS)
C
CONSTRUCT A GRAPHICAL DISPLAY ON THE LINEPRINTER
C
      CALL PRG(RES,50,5,IH,2,3,T,A4)
      CALL PRG(RES,50,5,IH,2,4,T,A4)
      CALL PRG(PES,50,5,IH,2,5,T,A4)
```

PRASEODYMIUM

```
      GOTO 300
  940 STOP
 1009 FORMAT(I1)
 1010 FORMAT(2F6.2)
 1012 FORMAT(F7.2)
 1008 FORMAT(I3)
 1011 FORMAT(2F7.2)
 2008 FORMAT(1H0,3X,6HTEMP K,5X,5HFIELD,5X,5HMAG C,5X,5HMAG H,5X
     A,7HAVERAGE)
 2000 FORMAT(1H0,22HFAILURE IN NAG F02 AMF)
 2001 FORMAT(1H0,37HEIGENVALUES HEXAGONAL SITES IN KELVIN)
 2002 FORMAT(1H0,26HCORRESPONDING EIGENVECTORS)
 2003 FORMAT(1H0,33HEIGENVALUES CUBIC SITES IN KELVIN)
 2004 FORMAT(1H1,11HRESULTS ARE)
 2005 FORMAT(1H0,25HAPPLIED FIELD IN TESLA IS)
 2006 FORMAT(1H+,28X,F8.2,14HIN X DIRECTION)
 2007 FORMAT(1H+,28X,F8.2,14HIN Z DIPECTION)
 2900 FORMAT(1H0,31HMAGNETIZATION IS NOT CONVERGING)
 2901 FORMAT(1H0,3HIH=,I3,3HIT=,I3,3HIM=,I3)
 1200 FORMAT(1H1,27HINPUT DATA FOR PRASEODYMIUM)
 1201 FORMAT(1H0,15HLOWEST FIELD IS,F8.2,6H TESLA)
 1202 FORMAT(1H0,9HTHERE ARE,I3,9H STEPS OF,F8.2,6H TESLA)
 1203 FORMAT(1H+,40X,22HAPPLIED IN X DIRECTION)
 1204 FORMAT(1H+,40X,22HAPPLIED IN Z DIRECTION)
 1205 FORMAT(1H0,32HMOLECULAR FIELD PARAMETERS USED=,2(F7.2,3X))
      END
      SUBROUTINE PRG(ROUT,NN,MM,NP,IX,IY,TT,A4)
      DIMENSION ROUT(NN,MM),ILINE(120),ICHAR(3)
      LOGICAL A4
      DATA ICHAR(1),ICHAR(2),ICHAR(3)/1H ,1H.,1H*/
      IF(NP.GT.NN) GOTO 900
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
CODE OUTPUTS A SIMPLE GRAPH OF ROUT ONTO LINEPRINTER
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      ILIM=120
      IF(A4) ILIM=71
      SMALL=10.0**(-10)
      RYM=ROUT(1,IY)
      RYS=0.0
      DO 100 II=1,NP
      IF(ROUT(II,IY).GT.RYM) RYM=ROUT(II,IY)
      IF(POUT(II,IY).LT.RYS) RYS=ROUT(II,IY)
  100 CONTINUE
      YB=RYS
      AYB=ABS(YB)
      IF(AYB.LT.SMALL) YB=0.0
      AYB=ABS(RYM-YB)
      IF(AYB.LT.SMALL) GOTO 900
      IF(.NOT.A4) RYS=109.0/(RYM-YB)
      IF(A4) RYS=69.0/(RYM-YB)
      IF(IY.EQ.3) GOTO 110
      IF(IY.EQ.4) GOTO 112
      WRITE(2,1902)
      GOTO 116
```

PRASEODYMIUM

```
  110 WRITE(2,1900)
      GOTO 116
  112 WRITE(2,1901)
  116 CONTINUE
      WRITE(2,1903) TT
      IF(IX.EQ.2) GOTO 120
      IF(IX.EQ.1) GOTO 122
      GOTO 130
  120 WRITE(2,2000)
      GOTO 130
  122 WRITE(2,2002)
  130 CONTINUE
  140 WRITE(2,2003)
      DO 320 II=1,ILIM
  320 ILINE(II)=ICHAR(2)
      IF(.NOT.A4) WRITE(2,2500) YB,RYM
      IF(A4) WRITE(2,2503) YB,RYM
      WRITE(2,2501)(ILINE(II),II=1,ILIM)
      RX=55.0/FLOAT(NP)
      ILX=IFIX(RX-0.50)
      DO 400 II=1,NP
      DO 360 JJ=1,ILIM
      ILINE(JJ)=ICHAR(1)
  360 CONTINUE
      ILINE(10)=ICHAR(2)
      Y=(ROUT(II,IY)-YB)*RYS
      Y=Y+0.50
      ILY=IFI/(Y)+10
      IF(ILY.GT.ILIM) ILY=ILIM
      ILINE(ILY)=ICHAR(3)
      WRITE(2,2501)(ILINE(JJ),JJ=1,ILIM)
      WRITE(2,2502) ROUT(II,IX)
      II INE(ILY)=ICHAR(1)
      ILINE(10)=ICHAR(2)
      IF(ILX.IE.1) GOIO 390
      DO 380 JJ=1,ILX
      WRITE(2,2501)(ILINE(KK),KK=1,ILIM)
  380 CONTINUE
  390 CONTINUE
  400 CONTINUE
 1900 FORMAT(1H1,20X,11HCUBIC SITES)
 1901 FORMAT(1H1,20X,15HHEXAGONAL SITES)
 1902 FORMAT(1H1,20X,23HAVERAGE FROM BOTH SITES)
 1903 FORMAT(1H ,40X,14HTEMPERATURE IS,F8.2,7H KELVIN)
 2000 FORMAT(1H0,12H FIELD TESLA)
 2002 FORMAT(1H0,11H TEM KELVIN)
 2003 FORMAT(1H+,50X,17HMAGNETISATION(BM))
C BM=BOHR MAGNETONS
 2500 FORMAT(1H ,10X,E10.2,90X,E10.2)
 2501 FORMAT(1H ,120A1)
 2502 FORMAT(1H+,F9.3)
 2503 FORMAT(1H ,10X,E10.2,28X,E10.2)

  900 RETURN
      END
      SUBROUTINE PRH(RH,CH,HX,HZ,B2,B4,B6)
```

```
PRASEODYMIUM


      DIMENSION RH(9,9)
      REAL B2,B4,B6,HX,HZ,H,G,X,XS,MU,SQP
      INTEGER CH
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
CONSTRUCTS THE HAMILTONIAN MATRICES FOR PRASEODYMIUM AND STORES IN RH
CH IS=0 FOR HEXAGONAL SITES AND=1 FOR CUBIC SITES
CONSTANTS B2 B4 B6 ARE THE THREE CRYSTAL FIELD PARAMETERS
CODE USES HX AND HZ FOR THE TOTAL MAGNETIC FIELDS IN X AND Z DIRE
CTIONS RESPECTIVELY.
C
      DO 100 I=1,9
      DO 100 J=1,9
  100 RH(I,J)=0.0
      RH(1,1)=28.0*B2+14.0*B4+4.0*B6+4.0*HZ
      RH(1,2)=SQRT(8.0)*HX
      RH(2,1)=RH(1,2)
      RH(8,9)=RH(1,2)
      RH(9,8)=RH(8,9)
      RH(1,7)=SQRT(7.0)*5.50*B6
      RH(7,1)=RH(1,7)
      RH(3,9)=RH(1,7)
      RH(9,3)=RH(3,9)
      RH(2,2)=7.0*B2-21.0*B4-17.0*B6+3.0*HZ
      RH(3,2)=SQRT(14.0)*HX
      RH(2,3)=RH(3,2)
      RH(7,8)=RH(2,3)
      RH(8,7)=RH(7,8)
      RH(2,8)=(77.0*B6)/4.0
      RH(8,2)=RH(2,8)
      RH(3,3)=-8.0*B2-11.0*B4+22.00*B6+2.0*HZ
      RH(3,4)=SQRT(18.0)*HX
      RH(4,3)=RH(3,4)
      RH(6,7)=RH(3,4)
      RH(7,6)=RH(6,7)
      RH(4,4)=-17.0*B2+9.0*B4+B6+HZ
      RH(4,5)=SQRT(20.0)*HX
      RH(5,4)=RH(4,5)
      RH(5,6)=RH(4,5)
      RH(6,5)=RH(5,6)
      RH(5,5)=-20.0*B2+18.0*B4-20.0*B6
      RH(6,6)=RH(4,4)-2.0*HZ
      RH(7,7)=RH(3,3)-4.0*HZ
      RH(8,8)=RH(2,2)-6.0*HZ
      RH(9,9)=RH(1,1)-8.0*HZ
      IF(CH.EQ.0) GOTO 900
C
CUBIC SYMMETRY TERMS ADDED NOW
C
      RH(1,4)=SQRT(7.0)*(10.0*B4-5.0*B6)
      RH(4,1)=RH(1,4)
      RH(2,5)=SQRT(70.0)*(3.0*B4+1.250*B6)
      RH(5,2)=RH(2,5)
      RH(3,6)=10.0*B4+8.750*B6
      RH(6,3)=RH(3,6)
```

PRASEODYMIUM

```
      RH(6,9)=-RH(1,4)
      RH(9,6)=RH(6,9)
      RH(5,8)=-RH(2,5)
      RH(8,5)=RH(5,8)
      RH(4,7)=-RH(3,6)
      RH(7,4)=RH(4,7)
  900 RETURN
      END
      SUBROUTINE PRINTM(RMAT,I1,I2,IPOW)
      DIMENSION RMAT(I1,I2)
C
COLUMNS OF MATRIX RMAT(I1,I2) PRINTED BY SUBROUTINE (MAX 12 COLS)
C
      LIM=I2
      IF(I2.GT.LIM) LIM=12
      IF(IROW.GT.I1) GOTO 910
      WRITE(2,2001)
      DO 100 II=1,IROW
      WRITE(2,2000)(RMAT(II,JJ),JJ=1,LIM)
  100 CONTINUE
      GOTO 900
  910 WRITE(2,2003) IROW,I1
 2000 FORMAT(1H ,12F10.4)
 2001 FORMAT(1H0)
 2003 FORMAT(1H0,24HPRINTM CALLED WITH IROW=,I6,5H  I1=,I6)
  900 RETURN
      END
      SUBROUTINE PRT(NN,EVEC,EVAL,TEM,ROP,RES)
      DIMENSION EVEC(NN,NN),EVAL(NN),ROP(NN,NN)
      DIMENSION RMOM(20),RU(20)
      REAL NUM,DEN
      INTEGER RR
      IF(NN.GT.20) GOTO 900
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
CALCULATES THE THERMAL AVERAGE OF AN OPERATOR ROP  GIVEN THE
CORECT EIGENVALUES STORED IN ASCENDING ORDER IN EVAL AND THE
CORRESPONDING EIGENVECTORS STORED IN EVEC.  TEM IS THE TEMPERATURE.
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      NUM=0.0
      DEN=0.0
      IF(TEM.LT.0.000000001) GOTO 800
      DO 100 II=1,20
      RMOM(II)=0.0
      RU(II)=0.0
  100 CONTINUE
      DO 200 KK=1,NN
      DO 110 II=1,NN
  110 RU(II)=0.0
      DO 160 II=1,NN
      DO 140 JJ=1,NN
      RU(II)=RU(II)+ROP(II,JJ)*EVEC(JJ,KK)
  140 CONTINUE
  160 CONTINUE
      DO 170 II=1,NN
```

PRASEODYMIUM

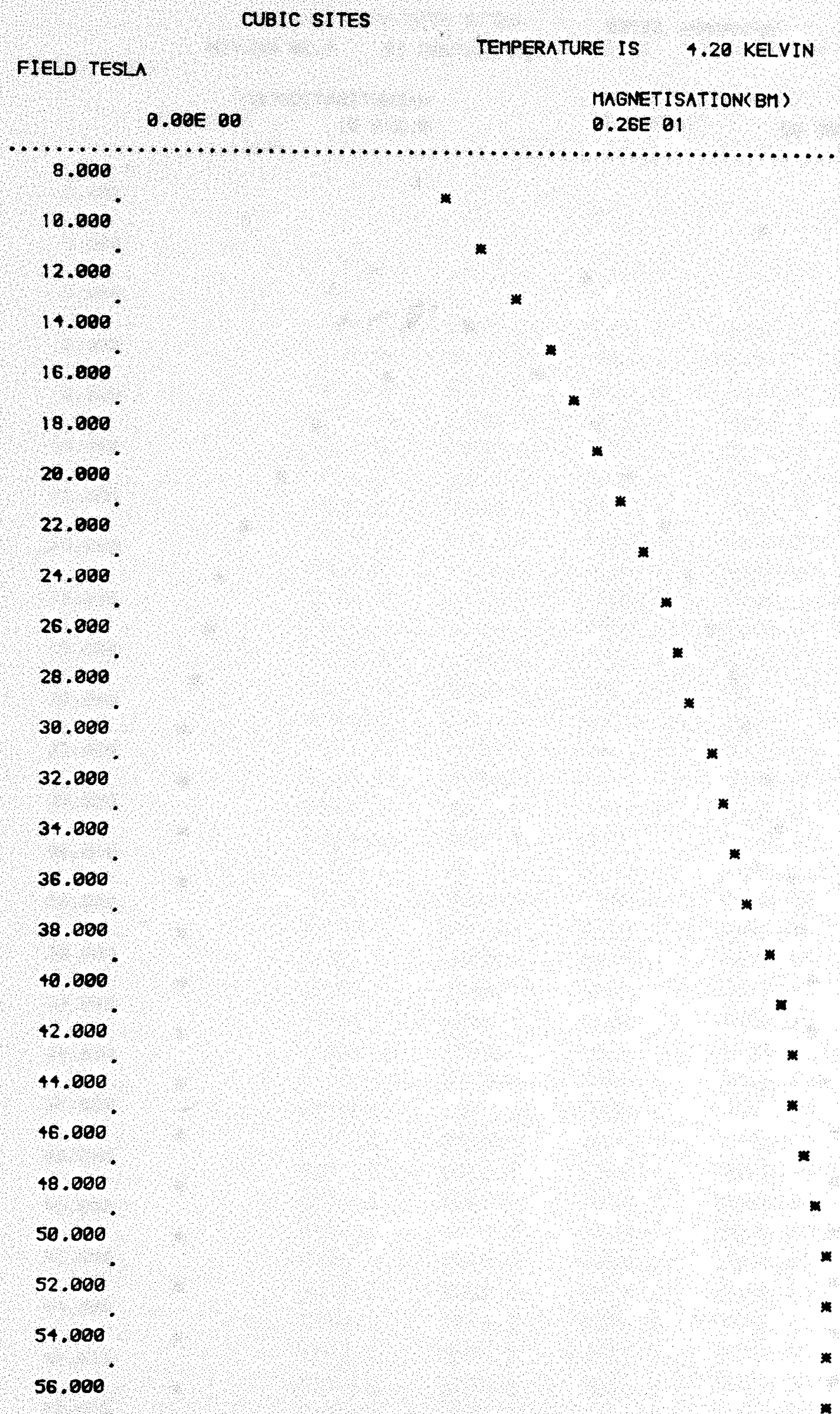
```
      RMOM(KK)=RMOM(KK)+EVEC(II,KK)*RU(II)
  170 CONTINUE
  200 CONTINUE
      NUM=EVAL(1)/TEM
      IF(NUM.LE.-60.0) GOTO 400
      NUM=0.0
      DO 210 II=1,NN
      XX=-EVAL(II)/TEM
      DEN=DEN+EXP(XX)
      NUM=NUM+RMOM(II)*EXP(XX)
  210 CONTINUE
      RES=NUM/DEN
      GOTO 900
  400 RR=0
      NUM=0.0
      DO 420 II=1,NN
  420 IF(EVAL(II).EQ.EVAL(1)) RR=RR+1
      DO 430 II=1,RR
  430 NUM=NUM+RMOM(II)
      JJ=RR+1
      XX=EVAL(RR)-EVAL(JJ)
      XX=EXP(XX/TEM)
      NUM=NUM+XX
      DEN=1.0+XX
      PES=NUM/DEN
      GOTO 900
  800 DO 820 II=1,20
      RMOM(II)=0.0
  820 RU(II)=0.0
      DO 830 II=1,NN
      DO 825 JJ=1,NN
  825 RU(II)=RU(II)+ROP(II,JJ)*EVEC(JJ,1)
  830 CONTINUE
      DO 840 II=1,NN
      RMOM(1)=RMOM(1)+EVEC(II,1)*RU(II)
  840 CONTINUE
      RES=RMOM(1)

      END
```

X DIRECTION RESULTS

```
INPUT DATA FOR PRASEODYMIUM
LOWEST FIELD IS     0.00 TESLA
THERE ARE 40 STEPS OF     2.00 TESLA
                                        APPLIED IN X DIRECTION
MOLECULAR FIELD PARAMETERS USED=  -1.20       4.14
RESULTS ARE
```

TEMP K	FIELD	MAG C	MAG H	AVERAGE
4.2000	0.0000	0.0000	-0.0000	0.0000
4.2000	2.0000	0.2789	0.5438	0.4113
4.2000	4.0000	0.5092	1.2042	0.8567
4.2000	6.0000	0.7421	1.6494	1.1957
4.2000	8.0000	0.9151	1.9961	1.4556
4.2000	10.0000	1.0634	2.2234	1.6434
4.2000	12.0000	1.1603	2.3644	1.7624
4.2000	14.0000	1.2907	2.5025	1.8966
4.2000	16.0000	1.3748	2.5829	1.9788
4.2000	18.0000	1.4722	2.6660	2.0691
4.2000	20.0000	1.5455	2.7167	2.1311
4.2000	22.0000	1.6143	2.7593	2.1868
4.2000	24.0000	1.6897	2.8080	2.2488
4.2000	26.0000	1.7500	2.8376	2.2938
4.2000	28.0000	1.8067	2.8635	2.3351
4.2000	30.0000	1.8601	2.8862	2.3732
4.2000	32.0000	1.9149	2.9141	2.4145
4.2000	34.0000	1.9622	2.9313	2.4467
4.2000	36.0000	2.0069	2.9467	2.4768
4.2000	38.0000	2.0493	2.9607	2.5050
4.2000	40.0000	2.0895	2.9734	2.5315
4.2000	42.0000	2.1289	2.9894	2.5591
4.2000	44.0000	2.1651	2.9996	2.5824
4.2000	46.0000	2.1997	3.0090	2.6044
4.2000	48.0000	2.2327	3.0177	2.6252
4.2000	50.0000	2.2642	3.0257	2.6449
4.2000	52.0000	2.2943	3.0332	2.6637
4.2000	54.0000	2.3232	3.0401	2.6816
4.2000	56.0000	2.3507	3.0492	2.6999
4.2000	58.0000	2.3773	3.0550	2.7162
4.2000	60.0000	2.4028	3.0605	2.7317
4.2000	62.0000	2.4275	3.0657	2.7466
4.2000	64.0000	2.4511	3.0705	2.7608
4.2000	66.0000	2.4740	3.0751	2.7745
4.2000	68.0000	2.4960	3.0794	2.7877
4.2000	70.0000	2.5173	3.0834	2.8004
4.2000	72.0000	2.5378	3.0873	2.8125
4.2000	74.0000	2.5570	3.0923	2.8247
4.2000	76.0000	2.5762	3.0957	2.8360
4.2000	78.0000	2.5948	3.0989	2.8468

X DIRECTION RESULTS



X DIRECTION RESULTS

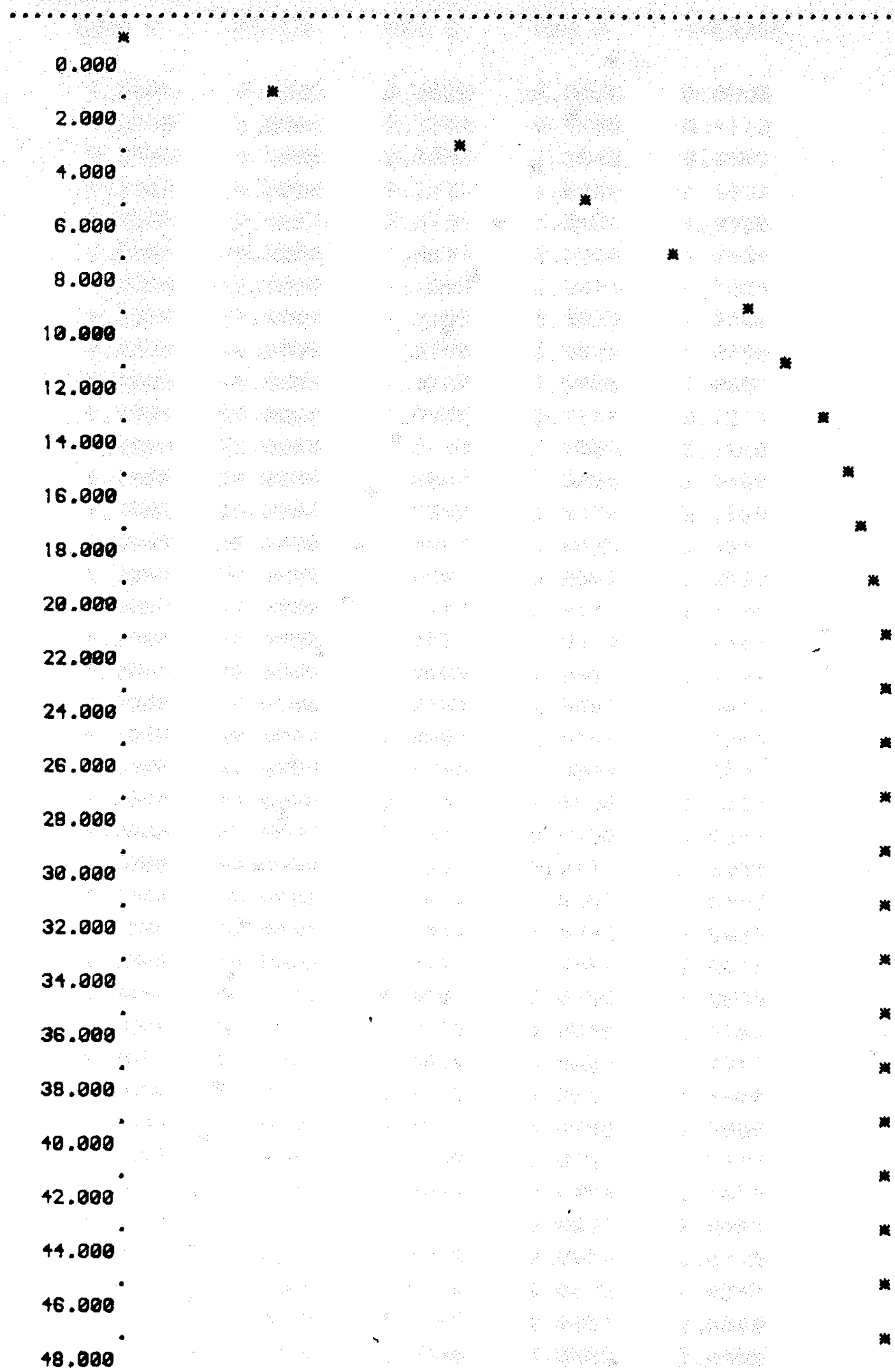
HEXAGONAL SITES

TEMPERATURE IS 4.20 KELVIN

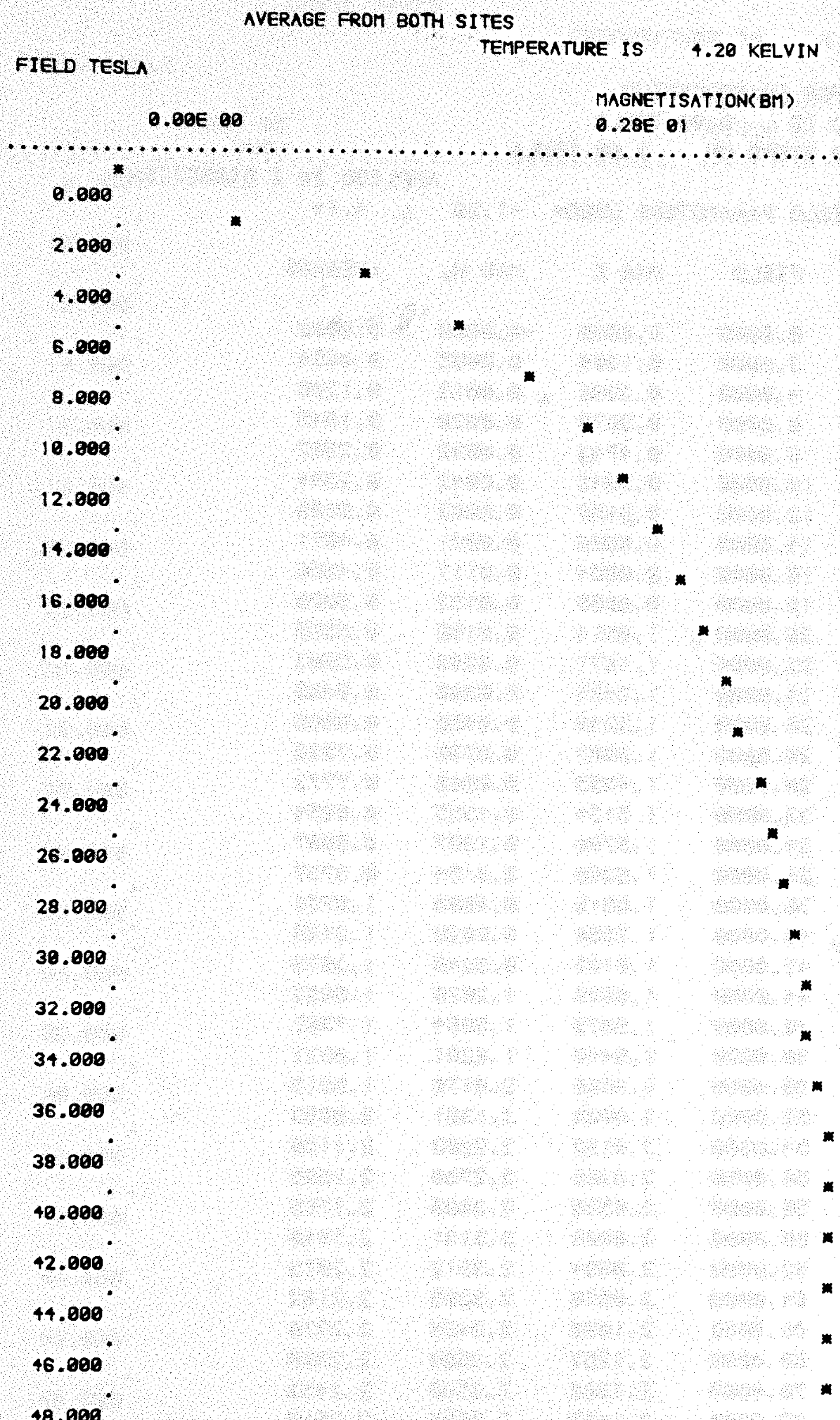
FIELD TESLA

MAGNETISATION(BM)

0.00E 00 0.31E 01



X DIRECTION RESULTS



Z DIRECTION RESULTS

INPUT DATA FOR PRASEODYMIUM
LOWEST FIELD IS 0.00 TESLA
THERE ARE 40 STEPS OF 2.00 TESLA
APPLIED IN Z DIRECTION
MOLECULAR FIELD PARAMETERS USED= -1.20 4.14
RESULTS ARE

TEMP K	FIELD	MAG C	MAG H	AVERAGE
4.2000	0.0000	0.0000	-0.0000	0.0000
4.2000	2.0000	0.1304	0.0005	0.0654
4.2000	4.0000	0.2398	0.0013	0.1206
4.2000	6.0000	0.3670	0.0020	0.1845
4.2000	8.0000	0.4743	0.0032	0.2387
4.2000	10.0000	0.5945	0.0042	0.2994
4.2000	12.0000	0.6956	0.0062	0.3509
4.2000	14.0000	0.8060	0.0081	0.4071
4.2000	16.0000	0.8994	0.0117	0.4556
4.2000	18.0000	0.9985	0.0152	0.5068
4.2000	20.0000	1.0914	0.0196	0.5555
4.2000	22.0000	1.1671	0.0293	0.5982
4.2000	24.0000	1.2485	0.0380	0.6433
4.2000	26.0000	1.3240	0.0496	0.6868
4.2000	28.0000	1.3907	0.0736	0.7322
4.2000	30.0000	1.4555	0.0988	0.7772
4.2000	32.0000	1.5154	0.1355	0.8254
4.2000	34.0000	1.5706	0.1907	0.8807
4.2000	36.0000	1.6360	0.3154	0.9757
4.2000	38.0000	1.6818	0.4683	1.0751
4.2000	40.0000	1.7556	0.6820	1.2188
4.2000	42.0000	1.8109	0.9649	1.3879
4.2000	44.0000	1.8628	1.2676	1.5652
4.2000	46.0000	1.9070	1.5664	1.7367
4.2000	48.0000	1.9440	1.8201	1.8821
4.2000	50.0000	1.9669	2.0170	1.9919
4.2000	52.0000	2.0003	2.1381	2.0692
4.2000	54.0000	2.0192	2.2203	2.1198
4.2000	56.0000	2.0369	2.2700	2.1535
4.2000	58.0000	2.0535	2.3003	2.1769
4.2000	60.0000	2.0689	2.3191	2.1940
4.2000	62.0000	2.0834	2.3312	2.2073
4.2000	64.0000	2.0970	2.3395	2.2182
4.2000	66.0000	2.1098	2.3454	2.2276
4.2000	68.0000	2.1257	2.3504	2.2380
4.2000	70.0000	2.1368	2.3538	2.2453
4.2000	72.0000	2.1472	2.3566	2.2519
4.2000	74.0000	2.1570	2.3591	2.2580
4.2000	76.0000	2.1663	2.3612	2.2638
4.2000	78.0000	2.1751	2.3632	2.2691

Z DIRECTION RESULTS

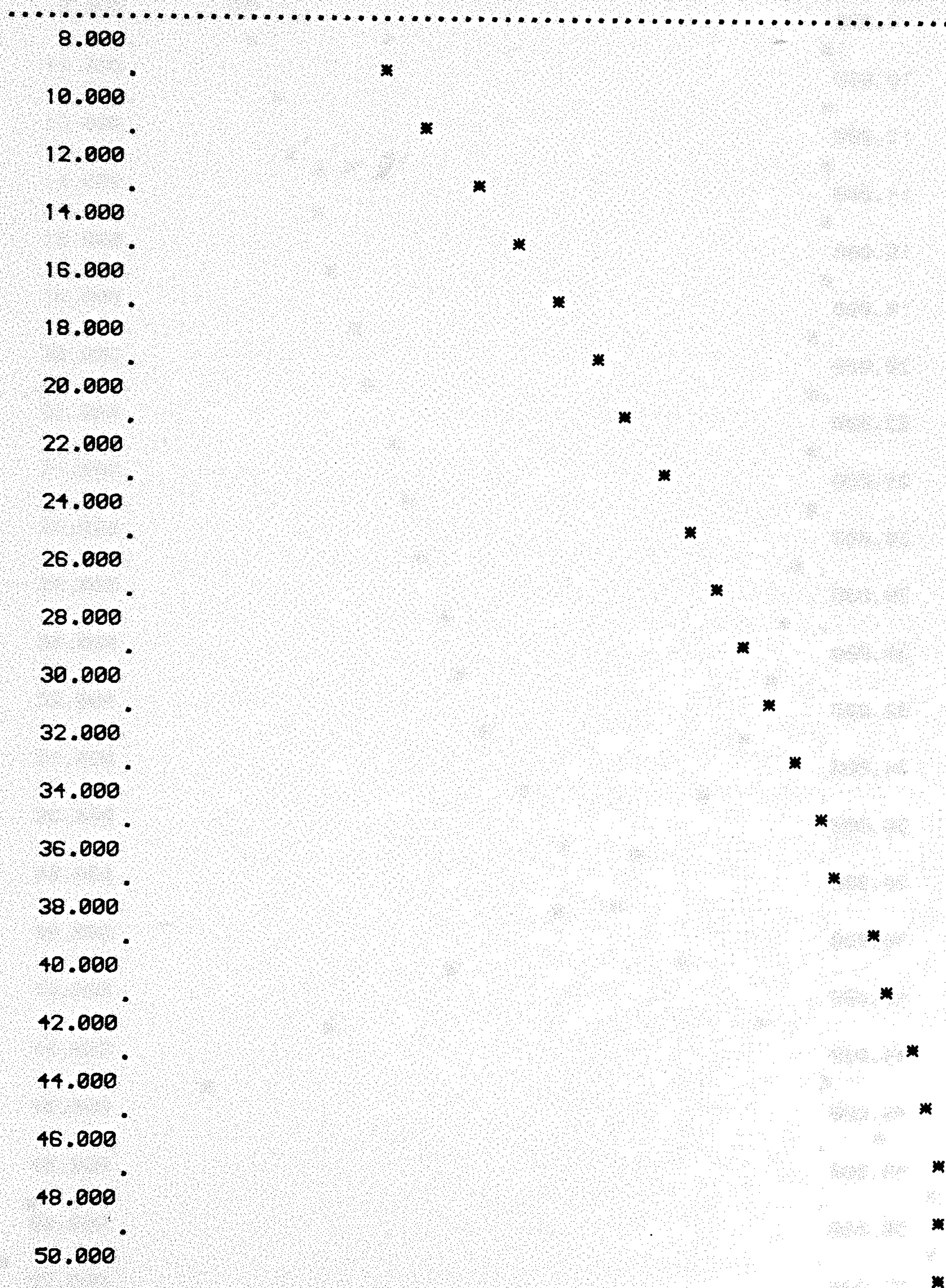
CUBIC SITES

TEMPERATURE IS 4.20 KELVIN

FIELD TESLA

MAGNETISATION(BM)

0.00E 00 0.22E 01



Z DIRECTION RESULTS

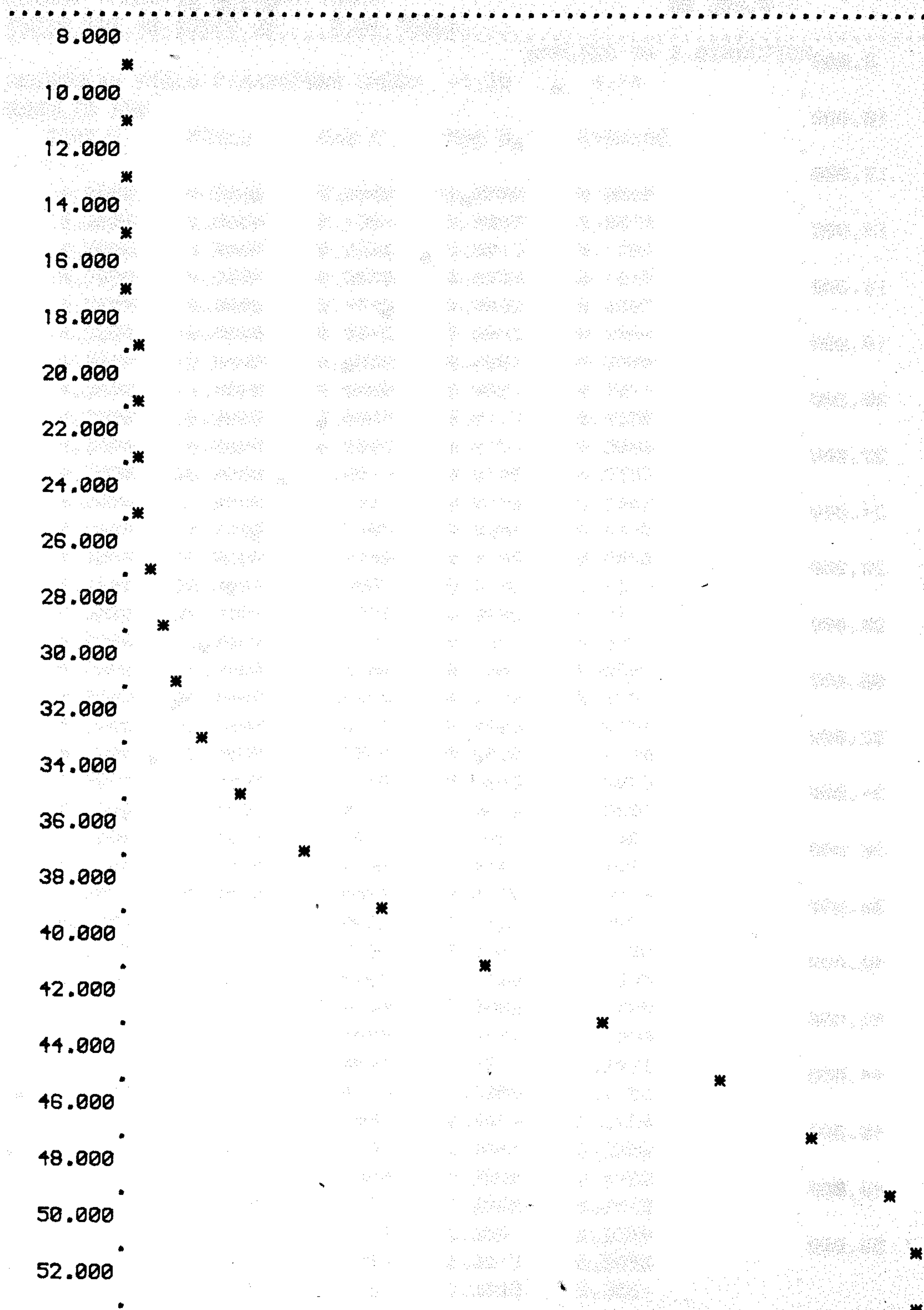
HEXAGONAL SITES

TEMPERATURE IS 4.20 KELVIN

FIELD TESLA

MAGNETISATION(BM)

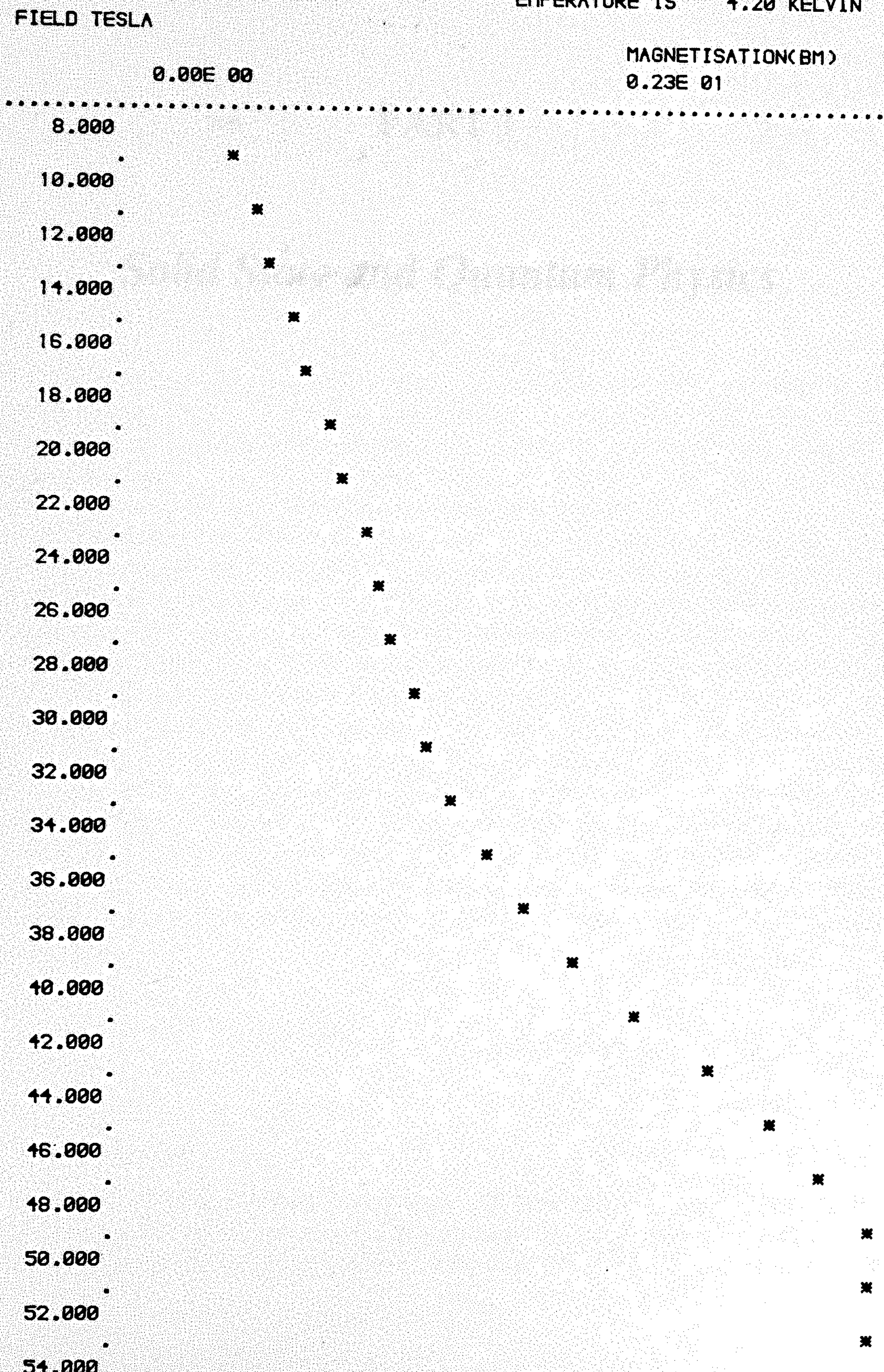
0.00E 00 0.24E 01



Z DIRECTION RESULTS

AVERAGE FROM BOTH SITES

TEMPERATURE IS 4.20 KELVIN



PART 3

Solid State and Quantum Physics

Physics Programs
Edited by A. D. Boardman

CHAPTER 7

Elastic Waves in Crystalline Solids

B. W. JAMES

1. INTRODUCTION

Several fundamental physical properties are related to the propagation of sound waves in solids and an understanding of these processes has led to the development of a number of devices. For example ultrasonic delay lines are widely used in colour television receivers, and diffraction grating dispersive filters are used in radar systems for pulse compression.

The behaviour of sound waves in gases, liquids, amorphous solids, and crystalline solids has been widely investigated. The study of the propagation of sound waves in crystalline solids is the most complex and most interesting of the forms of sound wave to investigate since account must be taken of the anisotropic elastic properties of crystalline solids (Love,[1] Musgrave,[2] and Pollard[3]). In each direction in a crystalline solid there will be three modes of propagation which will, in general, all have different phase velocities, particle motion directions, and energy flow directions. The largest velocity is associated with a longitudinal or nearly longitudinal wave and the other two velocities with transverse or nearly transverse waves. The particle motion directions of the three waves always form an orthogonal set. Pure longitudinal and transverse modes occur in high symmetry directions and in some accidental directions which may be obtained from the known physical properties.

2. TENSOR FORMULATION

2.1 Hooke's law

In order to discuss the elastic properties of anisotropic materials and hence the propagation of sound waves it is necessary to use a tensor formulation of Hooke's law as the stress and strain at a point are given by two second-rank tensors. Hence if σ_{ij} is the stress tensor and e_{kl} is the strain tensor then Hooke's law is written as

$$\sigma_{ij} = c_{ijkl} e_{kl} \quad (i, j, k, l = 1, 2, 3), \tag{1}$$

where c_{ijkl} is a fourth-rank tensor of 81 elements relating 9 stress components to 9 strain components. (Note that summation is assumed for repeated suffices, see Nye[4].)

2.2 The strain tensor

The particle displacements $\mathbf{U}$ of the strained material determine the nine elements of the general strain tensor E_{kl} and

$$E_{kl} = \frac{\partial U_k}{\partial x_l}, \tag{2}$$

where $\mathbf{U} = \mathbf{i}_1 U_1 + \mathbf{i}_2 U_2 + \mathbf{i}_3 U_3 = \mathbf{i}_i U_i$ and $\mathbf{i}_1, \mathbf{i}_2$, and $\mathbf{i}_3$ are unit vectors along the Cartesian axes x_1, x_2, and x_3 respectively.

The general tensor E_{kl} consists of a symmetrical part e_{kl} and an antisymmetrical part w_{kl}, where

$$e_{kl} = \frac{1}{2}\left(\frac{\partial U_k}{\partial x_l} + \frac{\partial U_l}{\partial x_k}\right), \tag{3}$$

and

$$w_{kl} = -\frac{1}{2}\left(\frac{\partial U_k}{\partial x_l} - \frac{\partial U_l}{\partial x_k}\right) = -w_{lk}. \tag{4}$$

Now if we first consider a rotation of the material about the origin of the axes without any deformation of the material, then in this rotation the displacement of any point is perpendicular to its radius vector so that

$$U_i x_i = 0 \quad \text{(scalar product)}, \tag{5}$$

or

$$E_{ij} x_i x_j = 0. \tag{6}$$

Since this is true for all x_i the coefficients on the left-hand side must all be zero. Hence

$$E_{ij} = 0 \quad \text{if } i = j; \qquad E_{ij} = -E_{ji} \quad \text{if } i \neq j, \tag{7}$$

which is just the condition for E_{ij} to be antisymmetrical. So that in the special case of a rotation of the material about the origin of the axes without deformation, the general strain tensor E_{kl} becomes antisymmetrical, with the rotation of the material about the origin of the axes given by the