Direct Determination of Crystal Structure

I. Monte Carlo Method

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Abstract

Electronic computer's program for direct determination of crystal structure by Monte Carlo Method is made for pyrenocine analyzed by Sato, Konoma, Sakumura, Furusaki, Matsumoto and Matsuzaki [Agri. Biol. Chem. 45, 795 (1981)]. The R-value for 316 strong reflections of the structure obtained from the structure with the smallest R-value among 61 structures which are obtained by using 52 reflections, becomes 0.27 by successive application of the method. The list of the program is shown.

1. Introduction

Direct determination of crystal structure has been discussed by many investigators in many respects. Although the author had been interested in the direct determination, he had no time to study sincerely the method. Recently, his paper concerning to critiscism against space-groupoid theory was rejected by the editor of Acta Crystallographica. Taking this opportunity, he formed a resolution to study the direct determination.

For the beginning of the study, the author read the review of Furusaki (1982) on Monte Carlo method applying to phase-determination. According to him, the method of Vand (1960) applying Monte Carlo method to the direct determination has the following defects,

(1) the probability hitting correct structure is too small,

(2) the corrections in optimal shift method are too large,

(3) there is no procedure correcting wrong structures.

The reason that the optimal shift method fails is very simple. If we suppose a very simple structure, Taylor series of the structure factor converges if $du_i=2\pi dx_i$ is less than 1.0. Unless the series converges for large dx_i, we can not obtain the structure factor by successive approximation. The defcts (1) and (3) can be avoided if we apply similar method with that of Metropolis (1953) in molecular dynamics.

Taking account of the recent development of electronic computer, the author judged

that crystal structures can be determined directly by Monte Carlo method. To compare with Furusaki's method, pyrenocine analyzed by Sato, Konoma, Sakumura, Furusaki, Matsumoto and Matsuzaki (1981), of which the coordinates of the atoms were informed by Furusaki (1983) was chosen as the testing material.

2. List of Program

The list of the program is shown at the last part of this paper. The program used at the 1st step of the calculation is as follows.

(1) The line 17 is deleted,

(2) the following line is inserted between the line 61 and 62,

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IF(NTRY. GT. 100) STOP
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(3) the following lines are inserted between the line 66 and 67,

```
DO 70 I=1, NA
DO 80 J=1, 3
CALL RANU2 (IX, RAN, 1, ICON)
A=0. 001*AINT(A)
GX(J, I)=HX(J, I)
80 CONTINUE
90 CONTINUE
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(4) the following lines are inserted between the line 122 and 123.

```
IF(NCAL. GE. 100. AND. RI. GE. 0. 2)  GO TO 69
IF(NCAL. GE. 300. AND. RI. GE. 0. 1)  GO TO 69
```

3. Result

In our calculation, the structure factors calculated with the coordinates of pyrenocine were used instead of observed intensities. The scattering factors were substituted for the atomic numbers. Suitable starting structures were searched by using 52 reflections with $|F(h)|>25.0$. After calculation of CPU time 1 hour by FACOM M382, we obtained 7 structures with $0.1\leq R<0.2$ and 1 structure with $R<0.1$ among 61 structures. Finaly we obtained the structure with $R=0.27$ starting from the structure with the smallest R-value by successive application of our calculation. The results are summarized in the following list.

	initial R	*final R*	*reflections*	$\|F\|$
1st step	0.728	0.063	52	25.0
2nd step	0.192	0.136	116	21.0
3rd step	0.227	0.215	196	18.0
4th step	0.285	0.271	316	15.0

4. Discussion

The change of the value of DX did not give any remarkable effect on the diminishing of R-value. The value DX is a constant and equal to 0.2 in the author's present program. The line 118 is to be revised to

IF (ARI. LE. 0.001) GO TO 300

and the line 123 is to be deleted.

The convergence of *R*-value is very rapid. We can see the tendency of the convergence at very small number of NCAL. In our example, the value of RI at NCAL=100 is 0.0856, but the final NCAL is 1100 in the first step. The decreasing of *R*-value becomes small, when the number of the reflections becomes large. If the number of reflections increases, CPU time increases very much compared with diminishing of *R*-value. Our method is not profitable for the large number of reflections. The coordinates of atoms can be determined if the number of independent reflections is larger than 6NA, where NA is the number of independent atoms in a unit cell. It is better to limit the number of reflections within slightly larger than 6NA in the final step, and to refine the coordinates by the other method for larger reflections.

The author wished to improve his program to obtain structures with small *R*-value at once. The attempt failed almost all. The *R*-value could be diminished, but the increase of CPU time became very large. It is better to stop calculation and to examine another structure, if *R*-value is larger than the value previously determined at a given NCAL. This is valid for the case of the refinement.

There are three kinds of ways for improvement of our calculation,

(A) to find more effective parameter than *R*-value,

(B) to make slow the convergence of *R*-value,

(C) to consider the set of reflections.

We can not find any parameter at present. There are two ways for the refinement concerning to (B). (1) The order of calculation between the line 125 and 185 is changed. This can be done by using random numbers. Although the result of the calculation by

the author did not show any effect, it should be effective for the refinement. (2) The calculattion between the line 125 and 188 alternates between that by using LNR reflections and that by using LNR*c reflections with large rh, $r\mathrm{h}=||E_o|-|E_c||/|E_o|$. In the author's example, R-value did not converge when $c=0.5$, and was improved considerably when $c=0.75$ and NCAL$=10n-50n$, but when NCAL$=5n$, R-value did not converge eventhough $c=0.75$. Eventhough (C) is not for the improvement of the program in the proper sense, it is very important for practical sense. We should choose lower order reflections in general.

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References

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000001          DOUBLE PRECISION PAIT,SC,SF,H,F,HF,AF,DF,AH,AK,AL,SUMF,SUMHF,
               1BB,ABB,CC,HX,SX,AX,AY,AZ,CX,CY,CZ,GF,SUMDF,RIS
000002          DIMENSION SC(100),F(1000),HF(1000),AF(1000),GF(1000),
               1X(3,100),HX(3,100),SX(3,100),IH(3,1000),H(3,1000),DF(1000),
               2RAN(1),RIS(100)
000003          PAIT=6.283185307179586
000004      510 FORMAT(8I10)
000005          WRITE(6,660)
000006          WRITE(6,655)
000007      655 FORMAT(///,5X,'CRYSTAL      STRUCTURE DETERMINATION BY REDUCING',
               1 ' R-VALUE')
          C     NR IS NUMBER OF TOTAL REFLECTIONS AND LNR IS NUMBER OF REFLECTIONS
          C     USED IN THIS CALCULATION
000008          READ(5,510)NA,NR
000009          WRITE(6,611)NA,NR
000010      611 FORMAT(///,5X,'NUMBER      OF ATOMS =',I5,/,
               15X,'NUMBER OF REFLECTIONS =',I5)
000011          WRITE(6,650)
000012      650 FORMAT(///,5X,'COORDINATES OF ATOMS')
000013          READ(5,501)(SC(J),(X(I,J),I=1,3),J=1,NA)
000014      501 FORMAT(2(F5.0,3F10.0))
000015          WRITE(6,601)(SC(J),(X(I,J),I=1,3),J=1,NA)
000016      601 FORMAT(2(5X,4F10.5))
000017          READ(5,501)(SC(J),(HX(I,J),I=1,3),J=1,NA)
000018          READ(5,511)((IH(I,J),I=1,3),J=1,NR)
000019      511 FORMAT(3I5)
000020          DO 10 I=1,NR
000021          DO 20 J=1,3
000022          H(J,I)=PAIT*IH(J,I)
000023       20 CONTINUE
000024       10 CONTINUE
000025          DO 30 I=1,NR
000026          F(I)=0.0
000027          AH=H(1,I)
000028          AK=H(2,I)
000029          AL=H(3,I)
000030          AHK=0.5*(IH(1,I)+IH(2,I))
000031          ALO=0.5*IH(3,I)
000032          CHK=AHK-AINT(AHK)
000033          CLO=ALO-AINT(ALO)
000034          DO 40 J=1,NA
000035          AX=X(1,J)
000036          AY=X(2,J)
000037          AZ=X(3,J)
000038          IF(ABS(CHK).LT.0.001.AND.ABS(CLO).LT.0.001) GO TO 41
000039          IF(ABS(CHK).LT.0.001.AND.ABS(CLO).GE.0.001) GO TO 42
000040          IF(ABS(CHK).GE.0.001.AND.ABS(CLO).LT.0.001) GO TO 43
000041          IF(ABS(CHK).GE.0.001.AND.ABS(CLO).GE.0.001) GO TO 44
000042       41 CONTINUE
000043          F(I)=F(I)+SC(J)*DCOS(AH*AX)*DCOS(AK*AY)*DCOS(AL*AZ)
000044          GO TO 40
000045       42 CONTINUE
000046          F(I)=F(I)-SC(J)*DCOS(AH*AX)*DSIN(AK*AY)*DSIN(AL*AZ)
000047          GO TO 40
000048       43 CONTINUE
000049          F(I)=F(I)-SC(J)*DSIN(AH*AX)*DCOS(AK*AY)*DSIN(AL*AZ)
000050          GO TO 40
000051       44 CONTINUE
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000052          F(I)=F(I)-SC(J)*DSIN(AH*AX)*DSIN(AK*AY)*DCOS(AL*AZ)
000053       40 CONTINUE
000054          AF(I)=DABS(F(I))
000055       30 CONTINUE
000056          READ(5,510)IX
000057          WRITE(6,615)IX
000058      615 FORMAT(/,5X,'INITIAL IX ='I10)
000059          NTRY=0
000060       69 CONTINUE
000061          NTRY=NTRY+1
000062          WRITE(6,660)
000063          WRITE(6,613)NTRY
000064      613 FORMAT(///,5X,'TRIAL NUMBER =',I5)
000065          WRITE(6,614)
000066      614 FORMAT(///,5X,'INITIAL COORDINATES')
000067          WRITE(6,601)(SC(J),(HX(I,J),I=1,3),J=1,NA)
000068          DX=0.2
000069          LNR=NR
000070          SUMF=0.0
000071          DO 90  I=1,LNR
000072          SUMF=SUMF+AF(I)
000073       90 CONTINUE
000074          NCAL=0
000075          NSTEP=0
000076      129 CONTINUE
000077          NSTEP=NSTEP+1
000078          SUMHF=0.0
000079          DO 130 I=1,LNR
000080          AH=H(1,I)
000081          AK=H(2,I)
000082          AL=H(3,I)
000083          AHK=0.5*(IH(1,I)+IH(2,I))
000084          ALO=0.5*IH(3,I)
000085          CHK=AHK-AINT(AHK)
000086          CLO=ALO-AINT(ALO)
000087          HF(I)=0.0
000088          DO 140 J=1,NA
000089          AX=HX(1,J)
000090          AY=HX(2,J)
000091          AZ=HX(3,J)
000092          IF(ABS(CHK).LT.0.001.AND.ABS(CLO).LT.0.001) GO TO 141
000093          IF(ABS(CHK).LT.0.001.AND.ABS(CLO).GE.0.001) GO TO 142
000094          IF(ABS(CHK).GE.0.001.AND.ABS(CLO).LT.0.001) GO TO 143
000095          IF(ABS(CHK).GE.0.001.AND.ABS(CLO).GE.0.001) GO TO 144
000096      141 CONTINUE
000097          HF(I)=HF(I)+SC(J)*DCOS(AH*AX)*DCOS(AK*AY)*DCOS(AL*AZ)
000098          GO TO 140
000099      142 CONTINUE
000100          HF(I)=HF(I)-SC(J)*DCOS(AH*AX)*DSIN(AK*AY)*DSIN(AL*AZ)
000101          GO TO 140
000102      143 CONTINUE
000103          HF(I)=HF(I)-SC(J)*DSIN(AH*AX)*DCOS(AK*AY)*DSIN(AL*AZ)
000104          GO TO 140
000105      144 CONTINUE
000106          HF(I)=HF(I)-SC(J)*DSIN(AH*AX)*DSIN(AK*AY)*DCOS(AL*AZ)
000107      140 CONTINUE
000108          GF(I)=HF(I)
000109          BB=DABS(HF(I))
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000110          CC=DABS(AF(I)-BB)
000111          SUMHF=SUMHF+CC
000112      130 CONTINUE
000113          RI=SUMHF/SUMF
000114          NS=NSTEP-1
000115          RIS(NSTEP)=RI
000116          IF(NS.EQ.0) GO TO 150
000117          ARI=ABS(RI-RIS(NS))
000118          IF(ARI.LE.0.001)DX=0.1*DX
000119      150 CONTINUE
000120          WRITE(6,602)NCAL,RI
000121      602 FORMAT(5X,I6,F10.5)
000122          WRITE(6,601)(SC(J),(HX(I,J),I=1,3),J=1,NA)
000123          IF(DX.LT.0.001) GO TO 300
000124      179 CONTINUE
000125          DO 200 I=1,NA
000126          SF=SC(I)
000127          DO 210 J=1,3
000128          AX=HX(1,I)
000129          AY=HX(2,I)
000130          AZ=HX(3,I)
000131          SX(1,I)=AX
000132          SX(2,I)=AY
000133          SX(3,I)=AZ
000134          CALL RANU2(IX,RAN,1,ICON)
000135          DO 220 II=1,5
000136          DO 230 JJ=1,2
000137          ADX=DX*II*(-1)**JJ
000138          ADX=ADX*RAN(1)
000139          SUMDF=0.0
000140          DO 240 K=1,LNR
000141          AHK=0.5*(IH(1,K)+IH(2,K))
000142          ALO=0.5*IH(3,K)
000143          CHK=AHK-AINT(AHK)
000144          CLO=ALO-AINT(ALO)
000145          AH=H(1,K)
000146          AK=H(2,K)
000147          AL=H(3,K)
000148          SX(J,I)=HX(J,I)+ADX
000149          CX=SX(1,I)
000150          CY=SX(2,I)
000151          CZ=SX(3,I)
000152          IF(ABS(CHK).LT.0.001.AND.ABS(CLO).LT.0.001) GO TO 251
000153          IF(ABS(CHK).LT.0.001.AND.ABS(CLO).GE.0.001) GO TO 252
000154          IF(ABS(CHK).GE.0.001.AND.ABS(CLO).LT.0.001) GO TO 253
000155          IF(ABS(CHK).GE.0.001.AND.ABS(CLO).GE.0.001) GO TO 254
000156      251 CONTINUE
000157          DF(K)=HF(K)+SF*(DCOS(AH*CX)*DCOS(AK*CY)*DCOS(AL*CZ)
                1-DCOS(AH*AX)*DCOS(AK*AY)*DCOS(AL*AZ))
000158          GO TO 255
000159      252 CONTINUE
000160          DF(K)=HF(K)-SF*(DCOS(AH*CX)*DSIN(AK*CY)*DSIN(AL*CZ)
                1-DCOS(AH*AX)*DSIN(AK*AY)*DSIN(AL*AZ))
000161          GO TO 255
000162      253 CONTINUE
000163          DF(K)=HF(K)-SF*(DSIN(AH*CX)*DCOS(AK*CY)*DSIN(AL*CZ)
                1-DSIN(AH*AX)*DCOS(AK*AY)*DSIN(AL*AZ))
000164          GO TO 255
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000165     254 CONTINUE
000166         DF(K)=HF(K)-SF*(DSIN(AH*CX)*DSIN(AK*CY)*DCOS(AL*CZ)
                1-DSIN(AH*AX)*DSIN(AK*AY)*DCOS(AL*AZ))
000167     255 CONTINUE
000168         BB=AF(K)-DABS(DF(K))
000169         ABB=DABS(BB)
000170         SUMDF=SUMDF+ABB
000171     240 CONTINUE
000172         IF(SUMDF.GE.SUMHF)  GO TO 230
000173         SUMHF=SUMDF
000174         HX(J,I)=SX(J,I)
000175         DO 260 K=1,LNR
000176         GF(K)=DF(K)
000177     260 CONTINUE
000178     230 CONTINUE
000179     220 CONTINUE
000180         HX(J,I)=HX(J,I)-DINT(HX(J,I))
000181         DO 270 K=1,LNR
000182         HF(K)=GF(K)
000183     270 CONTINUE
000184     210 CONTINUE
000185     200 CONTINUE
000186         NCAL=NCAL+1
000187         IF(MOD(NCAL,100).EQ.0) GO TO 129
000188         GO TO 179
000189     300 CONTINUE
000190         WRITE(6,660)
000191     660 FORMAT(1H1)
000192         WRITE(6,618)RI
000193     618 FORMAT(/,5X,'R =',F10.5)
000194         WRITE(6,656)NCAL
000195     656 FORMAT(/,5X,'NCAL =',I6)
000196         WRITE(6,652)
000197     652 FORMAT(/,5X,'HX(I),I=1,3),J=1,NA)')
000198         WRITE(6,601)(SC(J),(HX(I,J),I=1,3),J=1,NA)
000199         WRITE(6,653)
000200     653 FORMAT(///,5X,'COMPARISON BETWEEN FI AND HF')
000201         WRITE(6,654)
000202     654 FORMAT(/,5X,'     H     K     L          F          HF')
000203         LNRT=LNR/2
000204         DO 450 I=1,LNRT
000205         II=I+LNRT
000206         WRITE(6,603)IH(1,I),IH(2,I),IH(3,I),F(I),HF(I),
              1IH(1,II),IH(2,II),IH(3,II),F(II),HF(II)
000207     603 FORMAT(2(5X,3I5,5X,2F10.5))
000208     450 CONTINUE
000209         STOP
000210         END
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R = 0.27088

NCAL = 600

HX(I),I=1,3),J=1,NA)

6.00000	0.71199	-0.05934	0.91037	6.00000	0.09783	-0.53986	-0.40909
6.00000	-0.96971	0.09443	0.35812	6.00000	0.14873	0.58056	0.15406
6.00000	0.91594	0.38379	0.89969	8.00000	0.59930	0.13469	0.41039
8.00000	0.47160	0.56049	0.27381	8.00000	-0.73496	0.13723	0.63480
6.00000	0.97417	0.42753	-0.22885	6.00000	-0.02819	-0.94201	0.22782
6.00000	-0.41274	0.86091	0.99209	6.00000	0.71696	0.49314	-0.13170
6.00000	0.02786	-0.05943	-0.22846	6.00000	0.53330	-0.85232	0.53986
8.00000	-0.20732	0.76515	-0.01257				

COMPARISON BETWEEN FI AND HF

H	K	L	F	HF	H	K	L	F	HF
0	0	6	-25.09268	-14.95579	7	10	14	-17.78585	-17.80076
0	0	8	25.67503	36.30489	7	11	12	18.42698	-2.08140
0	0	14	21.11401	24.93284	8	1	4	36.52656	-36.15403
0	2	0	33.31723	27.29699	8	1	8	19.85971	2.87210
0	2	1	30.88285	-31.58985	8	1	10	-29.74365	32.80463
0	2	2	-25.18615	-26.02203	8	1	11	-33.80591	-34.02596
0	2	7	-26.85451	24.88287	8	1	12	39.28876	-46.17853
0	2	13	16.98445	-22.49849	8	1	14	-18.45007	3.98707
0	4	0	-26.12035	-21.76359	8	3	3	-19.56784	-27.68298
0	4	1	38.20701	-41.88622	8	3	5	22.02006	21.66073
0	4	2	-16.43562	-4.03786	8	3	6	-16.81631	2.72721
0	4	3	-22.56163	6.87509	8	3	10	-26.96322	22.53408
0	4	7	-20.80638	20.32627	8	3	11	-60.35148	-59.67865
0	4	9	15.78675	-9.28975	8	3	13	18.63689	18.63249
0	6	0	-17.60010	-21.55054	8	5	4	-22.91858	16.02275
0	6	1	25.27786	-22.48151	8	5	5	28.59382	27.08275
0	6	2	21.13388	19.12739	8	5	9	27.72992	32.30419
0	6	5	19.66276	-12.82512	8	5	11	-15.07119	-9.64434
0	6	6	17.54599	5.37118	8	5	12	-23.10377	23.96374
0	6	10	17.25061	1.25790	8	5	13	32.46067	36.68259
0	8	2	24.57188	37.57106	8	7	9	17.66455	9.75103
0	8	4	-23.22448	-22.65559	8	7	10	30.07034	-30.11983
0	8	6	27.65312	23.87571	8	7	12	-19.23164	20.89339
0	8	12	-17.74308	-4.03701	8	7	14	32.79320	-33.96154
0	10	3	21.03520	-24.71901	8	9	1	-15.42204	-8.82307
0	10	4	-26.90871	-26.95470	8	9	6	17.90573	-17.90585
0	12	3	23.58600	-23.62130	8	9	8	-19.24109	26.83257
0	12	5	-29.04481	31.19637	8	9	12	-17.06271	20.75206
0	12	10	-23.94357	-25.25570	8	9	13	-28.57053	-29.47929
0	12	12	-18.48149	-12.53172	8	9	14	17.86016	-17.92654
0	14	0	25.06842	37.69684	8	11	6	16.40082	-25.51929
0	14	3	-15.03015	-6.17394	8	11	11	21.22989	19.30361
0	14	4	17.48867	9.14095	8	13	1	17.01951	17.01826
0	14	5	-29.79658	32.20839	8	13	8	19.77828	-11.98213
0	14	8	23.30136	15.56136	8	13	14	-18.02881	22.77450
0	14	13	-15.98586	16.17413	9	1	4	16.00588	4.60941
1	0	2	-20.37270	-32.85221	9	1	5	15.47387	7.68795
1	0	6	18.36893	18.42010	9	1	10	18.91880	-14.02246
1	1	8	-15.52188	7.90685	9	2	9	-15.66012	29.89783
1	2	1	21.33176	-13.33262	9	3	5	19.45185	12.74663
1	4	2	16.63607	6.53905	9	3	8	-16.14765	10.32101
1	6	2	15.43821	-2.30137	9	3	9	-18.06576	-10.96841
1	7	0	-19.90821	-28.54316	9	3	13	23.42817	17.47341
1	7	4	21.95279	-14.42958	9	4	6	-15.31431	-1.68612
1	7	5	15.29501	-10.87221	9	5	7	-16.41087	-9.94095

1	8	3	23.18581	-2.56528
1	10	12	16.18983	10.15781
1	12	3	-17.22517	16.98199
1	13	3	-20.43496	-25.77362
1	14	11	-16.08753	17.88961
2	0	0	-22.88524	18.42358
2	0	4	-28.70527	27.11515
2	2	1	-23.95686	-25.71379
2	2	9	-17.55524	-11.21974
2	4	0	26.06121	-19.36756
2	4	1	-22.94025	-22.22041
2	4	5	-19.82125	-21.35546
2	6	0	19.81021	-14.30005
2	6	2	-25.95809	29.80885
2	6	3	28.94429	27.31686
2	6	8	19.40427	-15.63256
2	7	2	17.40882	-4.08711
2	7	12	-16.65872	21.60534
2	8	2	-26.00603	26.22573
2	8	10	-15.72816	12.92823
2	8	12	-19.61533	15.75577
2	10	0	18.43379	-11.96720
2	10	3	-21.72702	-22.96176
2	10	4	21.36436	-21.85715
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