

This is the second post in the series of my posts on how to write an XRD Pattern simulator using C.

In the [last post](#), I showed you guys how to calculate the atomic form factor, as that would be used now in the calculation of structure factor. Structure factor is going to help us in calculating the intensity of the peaks for the XRD pattern.

The structure factor is given by the following equation,

$$F_{hkl} = \sum_{j=1}^n f_n \exp(2\pi i(xh + yk + zl))$$

where f_n is the atomic form factor.

Which can also be written as,

$$F_{hkl} = F_{real} + iF_{imag}$$

where

$$F_{real} = \sum_{j=1}^n f_n \cos(2\pi(xh + yk + zl)),$$

$$F_{imag} = \sum_{j=1}^n f_n \sin(2\pi(xh + yk + zl))$$

Therefore, structure factor, F has a real part as well as an imaginary part.

As can be seen from the above equation, we need the atomic positions of non-equivalent atoms and the h, k, l indices for which the S.F. (F) is required. What is not evident in the above equation is that we would also need the value of theta as well as the atomic species. These are required for calculating f_n which is the atomic form factor. You can refer to my last post for more information.

I am posting here two versions of the same program. One would require command-line inputs for the no. of atoms, theta, hkl values, atomic species and their positions.

The other version reads the no. of atoms and the atomic positions from a text file called atomicPos.txt

Ver. 1 CODE:

```
/*Structure Factor calculator
```

```
By: Manas Sharma
```

```
mail: feedback@bragittoff.com
```

```
http://bragittoff.com
```

```
IG: @__physwhiz__ */
```

```
#include<stdio.h>
```

```
#include<string.h>
```

```
#include<math.h>
```

```
/*
```

```
The following function takes the value of q(scattering vector) in the range 0 to 25 (Angstrom)^-1
```

```
and the name of the atomic specie using the atomic symbols
```

```
and returns the atomic form factor at that q value.
```

```
*/
```

```
double formFactorCalc(double q, char specie[]){
```

```
    //variable that will store the resulting form factor
```

```
    double result;
```

```
    int i, found=0,n;
```

```
    //Necessary tables needed for the calculations in array form
```

```
    char elements[211][10]={"H", "H1-
```

```

", "He", "Li", "Li1+", "Be", "Be2+", "B", "C", "Cval", "N", "O", "O1-", "F", "F1-
", "Ne", "Na", "Na1+", "Mg", "Mg2+", "Al", "Al3+", "Si", "Si1+", "Si4+", "P", "S", "Cl", "Cl1-
", "Ar", "K", "K1+", "Ca", "Ca2+", "Sc", "Sc3+", "Ti", "Ti2+", "Ti3+", "Ti4+", "V", "V2+", "V3+", "V5+
", "Cr", "Cr2+", "Cr3+", "Mn", "Mn2+", "Mn3+", "Mn4+", "Fe", "Fe2+", "Fe3+", "Co", "Co2+", "Co3+", "Ni",
"Ni2+", "Ni3+", "Cu", "Cu1+", "Cu2+", "Zn", "Zn2+", "Ga", "Ga3+", "Ge", "Ge4+", "As", "Se", "Br",
"Br1-
", "Kr", "Rb", "Rb1+", "Sr", "Sr2+", "Y", "Y3+", "Zr", "Zr4+", "Nb", "Nb3+", "Nb5+", "Mo", "Mo3+", "Mo5+
", "Mo6+", "Tc", "Ru", "Ru3+", "Ru4+", "Rh", "Rh3+", "Rh4+", "Pd", "Pd2+", "Pd4+", "Ag", "Ag1+", "Ag2+
", "Cd", "Cd2+", "In", "In3+", "Sn", "Sn2+", "Sn4+", "Sb", "Sb3+", "Sb5+", "Te", "I", "I1-
", "Xe", "Cs", "Cs1+", "Ba", "Ba2+", "La", "La3+", "Ce", "Ce3+", "Ce4+", "Pr", "Pr3+", "Pr4+", "Nd", "Nd3+
", "Pm", "Pm3+", "Sm", "Sm3+", "Eu", "Eu2+", "Eu3+", "Gd", "Gd3+", "Tb", "Tb3+", "Dy", "Dy3+", "Ho", "Ho3+
", "Er", "Er3+", "Tm", "Tm3+", "Yb", "Yb2+", "Yb3+", "Lu", "Lu3+", "Hf", "Hf4+", "Ta", "Ta5+", "W", "W6+
", "Re", "Os", "Os4+", "Ir", "Ir3+", "Ir4+", "Pt", "Pt2+", "Pt4+", "Au", "Au1+", "Au3+", "Hg", "Hg1+
", "Hg2+", "Tl", "Tl1+", "Tl3+", "Pb", "Pb2+", "Pb4+", "Bi", "Bi3+", "Bi5+", "Po", "At", "Rn", "Fr", "Ra", "Ra2+
", "Ac", "Ac3+", "Th", "Th4+", "Pa", "U", "U3+", "U4+", "U6+", "Np", "Np3+", "Np4+", "Np6+", "Pu", "Pu3+
", "Pu4+", "Pu6+", "Am", "Cm", "Bk", "Cf"};

```

```

double a1[]={0.489918 , 0.897661 , 0.8734 , 1.1282 , 0.6968 , 1.5919 , 6.2603 ,
2.0545 , 2.31 , 2.26069 , 12.2126 , 3.0485 , 4.1916 , 3.5392 , 3.6322 , 3.9553 , 4.7626
, 3.2565 , 5.4204 , 3.4988 , 6.4202 , 4.17448 , 6.2915 , 5.66269 , 4.43918 , 6.4345 ,
6.9053 , 11.4604 , 18.2915 , 7.4845 , 8.2186 , 7.9578 , 8.6266 , 15.6348 , 9.189 ,
13.4008 , 9.7595 , 9.11423 , 17.7344 , 19.5114 , 10.2971 , 10.106 , 9.43141 , 15.6887 ,
10.6406 , 9.54034 , 9.6809 , 11.2819 , 10.8061 , 9.84521 , 9.96253 , 11.7695 , 11.0424
, 11.1764 , 12.2841 , 11.2296 , 10.338 , 12.8376 , 11.4166 , 10.7806 , 13.338 , 11.9475
, 11.8168 , 14.0743 , 11.9719 , 15.2354 , 12.692 , 16.0816 , 12.9172 , 16.6723 ,
17.0006 , 17.1789 , 17.1718 , 17.3555 , 17.1784 , 17.5816 , 17.5663 , 18.0874 , 17.776
, 17.9268 , 17.8765 , 18.1668 , 17.6142 , 19.8812 , 17.9163 , 3.7025 , 21.1664 ,
21.0149 , 17.8871 , 19.1301 , 19.2674 , 18.5638 , 18.5003 , 19.2957 , 18.8785 , 18.8545
, 19.3319 , 19.1701 , 19.2493 , 19.2808 , 19.1812 , 19.1643 , 19.2214 , 19.1514 ,
19.1624 , 19.1045 , 19.1889 , 19.1094 , 18.9333 , 19.6418 , 18.9755 , 19.8685 , 19.9644
, 20.1472 , 20.2332 , 20.2933 , 20.3892 , 20.3524 , 20.3361 , 20.1807 , 20.578 ,
20.2489 , 21.1671 , 20.8036 , 20.3235 , 22.044 , 21.3727 , 20.9413 , 22.6845 , 21.961 ,
23.3405 , 22.5527 , 24.0042 , 23.1504 , 24.6274 , 24.0063 , 23.7497 , 25.0709 , 24.3466
, 25.8976 , 24.9559 , 26.507 , 25.5395 , 26.9049 , 26.1296 , 27.6563 , 26.722 , 28.1819
, 27.3083 , 28.6641 , 28.1209 , 27.8917 , 28.9476 , 28.4628 , 29.144 , 28.8131 ,
29.2024 , 29.1587 , 29.0818 , 29.4936 , 28.7621 , 28.1894 , 30.419 , 27.3049 , 30.4156
, 30.7058 , 27.0059 , 29.8429 , 30.9612 , 16.8819 , 28.0109 , 30.6886 , 20.6809 ,
25.0853 , 29.5641 , 27.5446 , 21.3985 , 30.8695 , 31.0617 , 21.7886 , 32.1244 , 33.3689
, 21.8053 , 33.5364 , 34.6726 , 35.3163 , 35.5631 , 35.9299 , 35.763 , 35.215 , 35.6597
, 35.1736 , 35.5645 , 35.1007 , 35.8847 , 36.0228 , 35.5747 , 35.3715 , 34.8509 ,
36.1874 , 35.7074 , 35.5103 , 35.0136 , 36.5254 , 35.84 , 35.6493 , 35.1736 , 36.6706 ,
36.6488 , 36.7881 , 36.9185};

```

```

double a2[]={0.262003 , 0.565616 , 0.6309 , 0.7508 , 0.7888 , 1.1278 , 0.8849 ,
1.3326 , 1.02 , 1.56165 , 3.1322 , 2.2868 , 1.63969 , 2.6412 , 3.51057 , 3.1125 ,
3.1736 , 3.9362 , 2.1735 , 3.8378 , 1.9002 , 3.3876 , 3.0353 , 3.07164 , 3.20345 ,
4.1791 , 5.2034 , 7.1964 , 7.2084 , 6.7723 , 7.4398 , 7.4917 , 7.3873 , 7.9518 , 7.3679
, 8.0273 , 7.3558 , 7.62174 , 8.73816 , 8.23473 , 7.3511 , 7.3541 , 7.7419 , 8.14208 ,
7.3537 , 7.7509 , 7.81136 , 7.3573 , 7.362 , 7.87194 , 7.97057 , 7.3573 , 7.374 ,
7.3863 , 7.3409 , 7.3883 , 7.88173 , 7.292 , 7.4005 , 7.75868 , 7.1676 , 7.3573 ,
7.11181 , 7.0318 , 7.3862 , 6.7006 , 6.69883 , 6.3747 , 6.70003 , 6.0701 , 5.8196 ,
5.2358 , 6.3338 , 6.7286 , 9.6435 , 7.6598 , 9.8184 , 8.1373 , 10.2946 , 9.1531 ,
10.948 , 10.0562 , 12.0144 , 18.0653 , 13.3417 , 17.2356 , 18.2017 , 18.0992 , 11.175 ,
11.0948 , 12.9182 , 13.2885 , 13.1787 , 14.3501 , 14.1259 , 13.9806 , 15.5017 , 15.2096
, 14.79 , 16.6885 , 15.9719 , 16.2456 , 17.6444 , 17.2535 , 18.5596 , 18.1108 , 19.1005
, 19.0548 , 19.7131 , 19.0455 , 18.933 , 19.0302 , 19.0138 , 18.9949 , 18.997 , 19.0298

```

```
, 19.1062 , 19.1278 , 19.297 , 19.1136 , 19.599 , 19.3763 , 19.7695 , 19.559 , 19.8186
, 19.6697 , 19.7491 , 20.0539 , 19.6847 , 19.9339 , 19.6095 , 20.1108 , 19.4258 ,
20.2599 , 19.0886 , 19.9504 , 20.3745 , 19.0798 , 20.4208 , 18.2185 , 20.3271 , 17.6383
, 20.2861 , 17.294 , 20.0994 , 16.4285 , 19.7748 , 15.8851 , 19.332 , 15.4345 , 17.6817
, 18.7614 , 15.2208 , 18.121 , 15.1726 , 18.4601 , 15.2293 , 18.8407 , 15.43 , 19.3763
, 15.7189 , 16.155 , 15.2637 , 16.7296 , 15.862 , 15.5512 , 17.7639 , 16.7224 , 15.9829
, 18.5913 , 17.8204 , 16.9029 , 19.0417 , 18.4973 , 18.06 , 19.1584 , 20.4723 , 18.3481
, 13.0637 , 19.5682 , 18.8003 , 12.951 , 19.5026 , 25.0946 , 15.4733 , 19.0211 ,
21.2816 , 23.0547 , 22.9064 , 21.67 , 23.1032 , 22.1112 , 23.4219 , 22.4418 , 23.2948 ,
23.4128 , 22.5259 , 22.5326 , 22.7584 , 23.5964 , 22.613 , 22.5787 , 22.7286 , 23.8083
, 22.7169 , 22.646 , 22.7181 , 24.0992 , 24.4096 , 24.7736 , 25.1995};
```

```
double a3[]={0.196767 , 0.415815 , 0.3112 , 0.6175 , 0.3414 , 0.5391 , 0.7993 ,
1.0979 , 1.5886 , 1.05075 , 2.0125 , 1.5463 , 1.52673 , 1.517 , 1.26064 , 1.4546 ,
1.2674 , 1.3998 , 1.2269 , 1.3284 , 1.5936 , 1.20296 , 1.9891 , 2.62446 , 1.19453 ,
1.78 , 1.4379 , 6.2556 , 6.5337 , 0.6539 , 1.0519 , 6.359 , 1.5899 , 8.4372 , 1.6409 ,
1.65943 , 1.6991 , 2.2793 , 5.25691 , 2.01341 , 2.0703 , 2.2884 , 2.15343 , 2.03081 ,
3.324 , 3.58274 , 2.87603 , 3.0193 , 3.5268 , 3.56531 , 2.76067 , 3.5222 , 4.1346 ,
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5.78135 , 5.1652 , 6.4668 , 4.3591 , 6.06692 , 3.7068 , 6.06791 , 3.4313 , 3.9731 ,
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5.41732 , 1.01118 , 4.04183 , 11.0177 , 10.799 , 12.8876 , 11.7423 , 11.4632 , 6.57891
, 4.64901 , 4.86337 , 9.32602 , 4.71304 , 4.73425 , 3.32515 , 2.53464 , 5.29537 ,
4.32234 , 2.89289 , 4.8045 , 5.27475 , 4.3709 , 4.461 , 4.47128 , 4.2948 , 3.78897 ,
4.4585 , 4.5648 , 3.4182 , 5.0371 , 5.10789 , 2.41253 , 6.14487 , 7.5138 , 7.8069 ,
8.9767 , 10.662 , 10.2821 , 10.888 , 10.9054 , 11.3727 , 11.6323 , 11.8513 , 11.9369 ,
12.1233 , 12.3856 , 12.1329 , 12.4668 , 12.774 , 12.12 , 13.1235 , 12.0671 , 13.4396 ,
11.9202 , 13.7603 , 11.8034 , 11.8509 , 13.8518 , 11.8708 , 14.3167 , 12.2471 , 14.5596
, 11.9812 , 14.5583 , 11.9788 , 14.9779 , 12.1506 , 15.1542 , 12.3339 , 15.3087 ,
13.3335 , 12.6072 , 15.1 , 12.8429 , 14.7586 , 12.7285 , 14.5135 , 12.8268 , 14.4327 ,
13.0544 , 14.5564 , 14.9305 , 14.7458 , 15.6115 , 13.6145 , 14.2326 , 15.7131 , 13.2153
, 13.7348 , 25.5582 , 14.3359 , 12.7801 , 21.6575 , 16.8883 , 12.8374 , 15.538 ,
18.7478 , 11.9328 , 18.442 , 19.1406 , 12.0175 , 16.5877 , 19.1053 , 19.2497 , 13.1138
, 9.49887 , 8.0037 , 12.1439 , 12.4739 , 7.91342 , 12.5977 , 8.19216 , 12.7473 ,
9.78554 , 14.1891 , 14.9491 , 12.2165 , 12.0291 , 14.0099 , 15.6402 , 12.9898 , 12.7766
, 14.3884 , 16.7707 , 13.5807 , 13.3595 , 14.7635 , 17.3415 , 17.399 , 17.8919 ,
18.3317};
```

```
double a4[]={0.049879 , 0.116973 , 0.178 , 0.4653 , 0.1563 , 0.7029 , 0.1647 ,
0.7068 , 0.865 , 0.839259 , 1.1663 , 0.867 , -20.307 , 1.0243 , 0.940706 , 1.1251 ,
1.1128 , 1.0032 , 2.3073 , 0.8497 , 1.9646 , 0.528137 , 1.541 , 1.3932 , 0.41653 ,
1.4908 , 1.5863 , 1.6455 , 2.3386 , 1.6442 , 0.8659 , 1.1915 , 1.0211 , 0.8537 , 1.468
, 1.57936 , 1.9021 , 0.087899 , 1.92134 , 1.5208 , 2.0571 , 0.0223 , 0.016865 , -9.576
, 1.4922 , 0.509107 , 0.113575 , 2.2441 , 0.2184 , 0.323613 , 0.054447 , 2.3045 ,
0.4399 , 0.0724 , 2.3488 , 0.7108 , 0.725591 , 2.38 , 0.9773 , 0.847114 , 1.6735 ,
1.5578 , 1.14523 , 2.41 , 1.394 , 2.9623 , 1.0066 , 3.683 , 0.859041 , 4.2779 , 4.3543
, 3.9851 , 3.7272 , 3.5375 , 1.5292 , 2.7817 , 2.6694 , -34.193 , 3.26588 , -33.108 ,
3.65721 , -2.6479 , 3.53346 , 1.94715 , 0.337905 , 3.7429 , 2.30951 , 0.740625 , 0 ,
2.71263 , 1.56756 , 3.00964 , 2.18535 , 1.28918 , -6.1989 , -5.6526 , 0.605844 , 0 ,
-7.9492 , 1.0463 , 0.357534 , 0 , 1.6029 , 0 , 2.0396 , 0 , 2.4663 , 0.487 , 0.0193 ,
2.6827 , 0.288753 , 0 , 2.5239 , 2.2735 , 2.8868 , 1.99 , 1.4953 , 0.9615 , 2.6959 ,
0.77634 , 3.28719 , 0.336048 , 3.33049 , 0.612376 , 0.144583 , 2.82428 , 0.97518 ,
0.296689 , 2.85137 , 1.51031 , 2.87516 , 2.07492 , 2.89604 , 2.71488 , 2.9227 , 3.87243
, 3.26503 , 3.54545 , 3.7149 , 2.95354 , 3.773 , 2.96577 , 4.50073 , 3.63837 , 4.93676
, 2.98233 , 5.17379 , 2.98706 , 5.38348 , 2.98963 , 5.14657 , 5.47647 , 3.71601 ,
5.59415 , 4.30013 , 5.59927 , 4.76492 , 5.38695 , 5.11982 , 5.06412 , 5.44174 , 5.67589
```

```

, 5.06795 , 5.83377 , 5.82008 , 5.53672 , 5.7837 , 6.35234 , 5.92034 , 5.86 , 6.58077 ,
6.52354 , 5.9676 , 6.48216 , 6.89912 , 5.52593 , 6.82847 , 7.00574 , 5.9696 , 7.01107 ,
6.96886 , 6.4692 , 7.10295 , 6.91555 , 7.02588 , 7.42518 , 7.4433 , 2.11253 , 3.21097 ,
7.65078 , 4.08655 , 7.05545 , 4.80703 , 5.29444 , 4.17287 , 4.188 , 5.37073 , 4.7984 ,
1.21457 , 4.1855 , 5.43227 , 4.92159 , 1.75669 , 3.47947 , 5.66016 , 5.18831 , 2.28678
, 3.49331 , 4.21665 , 4.23284 , 4.24391};
double b1[]={20.6593 , 53.1368 , 9.1037 , 3.9546 , 4.6237 , 43.6427 , 0.0027 ,
23.2185 , 20.8439 , 22.6907 , 0.0057 , 13.2771 , 12.8573 , 10.2825 , 5.27756 , 8.4042 ,
3.285 , 2.6671 , 2.8275 , 2.1676 , 3.0387 , 1.93816 , 2.4386 , 2.6652 , 1.64167 ,
1.9067 , 1.4679 , 0.0104 , 0.0066 , 0.9072 , 12.7949 , 12.6331 , 10.4421 , -0.0074 ,
9.0213 , 0.29854 , 7.8508 , 7.5243 , 0.22061 , 0.178847 , 6.8657 , 6.8818 , 6.39535 ,
0.679003 , 6.1038 , 5.66078 , 5.59463 , 5.3409 , 5.2796 , 4.91797 , 4.8485 , 4.7611 ,
4.6538 , 4.6147 , 4.2791 , 4.1231 , 3.90969 , 3.8785 , 3.6766 , 3.5477 , 3.5828 ,
3.3669 , 3.37484 , 3.2655 , 2.9946 , 3.0669 , 2.81262 , 2.8509 , 2.53718 , 2.6345 ,
2.4098 , 2.1723 , 2.2059 , 1.9384 , 1.7888 , 1.7139 , 1.5564 , 1.4907 , 1.4029 ,
1.35417 , 1.27618 , 1.2148 , 1.18865 , 0.019175 , 1.12446 , 0.2772 , 0.014734 ,
0.014345 , 1.03649 , 0.864132 , 0.80852 , 0.847329 , 0.844582 , 0.751536 , 0.764252 ,
0.760825 , 0.698655 , 0.696219 , 0.683839 , 0.6446 , 0.646179 , 0.645643 , 0.5946 ,
0.597922 , 0.5476 , 0.551522 , 5.8303 , 0.5036 , 5.764 , 5.3034 , 0.467196 , 5.44853 ,
4.81742 , 4.347 , 4.3579 , 3.9282 , 3.569 , 3.552 , 3.216 , 3.21367 , 2.94817 , 2.9207
, 2.81219 , 2.77691 , 2.65941 , 2.77393 , 2.6452 , 2.54467 , 2.66248 , 2.52722 , 2.5627
, 2.4174 , 2.47274 , 2.31641 , 2.3879 , 2.27783 , 2.22258 , 2.25341 , 2.13553 , 2.24256
, 2.05601 , 2.1802 , 1.9804 , 2.07051 , 1.91072 , 2.07356 , 1.84659 , 2.02859 , 1.78711
, 1.9889 , 1.78503 , 1.73272 , 1.90182 , 1.68216 , 1.83262 , 1.59136 , 1.77333 ,
1.50711 , 1.72029 , 1.42755 , 1.67191 , 1.62903 , 1.37113 , 1.59279 , 1.34323 , 1.30923
, 1.51293 , 1.32927 , 1.24813 , 0.4611 , 1.35321 , 1.2199 , 0.545 , 1.39507 , 1.21152 ,
0.65515 , 1.4711 , 1.1008 , 0.6902 , 1.3366 , 1.00566 , 0.704 , 1.2356 , 0.91654 ,
0.700999 , 0.68587 , 0.6631 , 0.646453 , 0.616341 , 0.604909 , 0.589092 , 0.579689 ,
0.563359 , 0.555054 , 0.547751 , 0.5293 , 0.52048 , 0.516598 , 0.507079 , 0.511929 ,
0.502322 , 0.498626 , 0.48981 , 0.499384 , 0.484938 , 0.481422 , 0.473204 , 0.483629 ,
0.465154 , 0.451018 , 0.437533};
double b2[]={7.74039 , 15.187 , 3.3568 , 1.0524 , 1.9557 , 1.8623 , 0.8313 ,
1.021 , 10.2075 , 0.656665 , 9.8933 , 5.7011 , 4.17236 , 4.2944 , 14.7353 , 3.4262 ,
8.8422 , 6.1153 , 79.2611 , 4.7542 , 0.7426 , 4.14553 , 32.3337 , 38.6634 , 3.43757 ,
27.157 , 22.2151 , 1.1662 , 1.1717 , 14.8407 , 0.7748 , 0.7674 , 0.6599 , 0.6089 ,
0.5729 , 7.9629 , 0.5 , 0.457585 , 7.04716 , 6.67018 , 0.4385 , 0.4409 , 0.383349 ,
5.40135 , 0.392 , 0.344261 , 0.334393 , 0.3432 , 0.3435 , 0.294393 , 0.283303 , 0.3072
, 0.3053 , 0.3005 , 0.2784 , 0.2726 , 0.238668 , 0.2565 , 0.2449 , 0.22314 , 0.247 ,
0.2274 , 0.244078 , 0.2333 , 0.2031 , 0.2412 , 0.22789 , 0.2516 , 0.205855 , 0.2647 ,
0.2726 , 16.5796 , 19.3345 , 16.5623 , 17.3151 , 14.7957 , 14.0988 , 12.6963 , 12.8006
, 11.2145 , 11.916 , 10.1483 , 11.766 , 1.13305 , 0.028781 , 1.0958 , 1.03031 , 1.02238
, 8.48061 , 8.14487 , 8.43467 , 8.37164 , 8.12534 , 8.21758 , 7.84438 , 7.62436 ,
7.98929 , 7.55573 , 7.14833 , 7.4726 , 7.19123 , 7.18544 , 6.9089 , 6.80639 , 6.3776 ,
6.3247 , 0.5031 , 5.8378 , 0.4655 , 0.4607 , 5.22126 , 0.467973 , 0.420885 , 0.3814 ,
0.3815 , 0.344 , 0.3107 , 0.3086 , 0.2756 , 0.28331 , 0.244475 , 0.250698 , 0.226836 ,
0.23154 , 0.21885 , 0.222087 , 0.214299 , 0.202481 , 0.210628 , 0.199237 , 0.202088 ,
0.185769 , 0.196451 , 0.174081 , 0.1942 , 0.17353 , 0.16394 , 0.181951 , 0.155525 ,
0.196143 , 0.149525 , 0.202172 , 0.143384 , 0.19794 , 0.139358 , 0.223545 , 0.13729 ,
0.238849 , 0.136974 , 0.257119 , 0.15997 , 0.13879 , 9.98519 , 0.142292 , 9.5999 ,
0.128903 , 9.37046 , 0.116741 , 9.2259 , 0.104621 , 9.09227 , 8.97948 , 6.84706 ,
8.86553 , 7.10909 , 6.71983 , 8.81174 , 7.38979 , 6.60834 , 8.6216 , 7.7395 , 6.82872 ,
8.4484 , 7.65105 , 7.05639 , 8.70751 , 0.517394 , 6.53852 , 2.3576 , 0.488383 , 6.10926
, 2.9238 , 6.24149 , 0.39042 , 3.55078 , 3.97458 , 4.0691 , 4.17619 , 3.87135 , 3.5767
, 3.65155 , 3.41437 , 3.46204 , 3.24498 , 3.41519 , 3.3253 , 3.12293 , 3.05053 , 2.8903

```

```

, 3.25396 , 3.03807 , 2.96627 , 2.81099 , 3.26371 , 2.96118 , 2.8902 , 2.73848 ,
3.20647 , 3.08997 , 3.04619 , 3.00775};
    double b3[]={49.5519 , 186.576 , 22.9276 , 85.3905 , 0.6316 , 103.483 , 2.2758
, 60.3498 , 0.5687 , 9.75618 , 28.9975 , 0.3239 , 47.0179 , 0.2615 , 0.442258 , 0.2306
, 0.3136 , 0.2001 , 0.3808 , 0.185 , 31.5472 , 0.228753 , 0.6785 , 0.916946 , 0.2149 ,
0.526 , 0.2536 , 18.5194 , 19.5424 , 43.8983 , 213.187 , -0.002 , 85.7484 , 10.3116 ,
136.108 , -0.28604 , 35.6338 , 19.5361 , -0.15762 , -0.29263 , 26.8938 , 20.3004 ,
15.1908 , 9.97278 , 20.2626 , 13.3075 , 12.8288 , 17.8674 , 14.343 , 10.8171 , 10.4852
, 15.3535 , 12.0546 , 11.6729 , 13.5359 , 10.2443 , 8.35583 , 12.1763 , 8.873 , 7.64468
, 11.3966 , 8.6625 , 7.9876 , 10.3163 , 7.0826 , 10.7805 , 6.36441 , 11.4468 , 5.47913
, 12.9479 , 15.2372 , 0.2609 , 0.2871 , 0.2261 , 0.2748 , 0.1603 , 0.1664 , 24.5651 ,
0.125599 , 22.6599 , 0.117622 , 21.6054 , 0.204785 , 10.1621 , 9.28206 , 11.004 ,
9.53659 , 8.78809 , 0.058881 , 21.5707 , 24.7997 , 0.017662 , 0.36495 , 25.8749 ,
21.2487 , 19.3317 , 25.2052 , 22.5057 , 17.9144 , 24.6605 , 21.7326 , 21.4072 , 24.7008
, 20.2521 , 25.8499 , 17.3595 , 26.8909 , 23.3752 , 14.0049 , 27.9074 , 19.5902 ,
14.1259 , 28.5284 , 27.766 , 29.5259 , 26.4659 , 24.3879 , 23.7128 , 20.2073 , 20.0558
, 18.7726 , 17.8211 , 17.6083 , 16.5408 , 15.7992 , 16.7669 , 15.323 , 14.8137 , 15.885
, 14.1783 , 15.1009 , 13.1275 , 14.3996 , 12.1571 , 13.7546 , 11.6096 , 11.311 ,
12.9331 , 10.5782 , 12.6648 , 10.0499 , 12.1899 , 9.34972 , 11.4407 , 8.80018 , 11.3604
, 8.36225 , 10.9975 , 7.96778 , 10.6647 , 8.18304 , 7.64412 , 0.261033 , 7.33727 ,
0.275116 , 6.76232 , 0.295977 , 6.31524 , 0.321703 , 5.93667 , 0.3505 , 0.382661 ,
0.165191 , 0.417916 , 0.204633 , 0.167252 , 0.424593 , 0.263297 , 0.16864 , 1.4826 ,
0.356752 , 0.212867 , 1.5729 , 0.443378 , 0.284738 , 1.96347 , 7.43463 , 0.219074 ,
8.618 , 6.7727 , 0.147041 , 8.7937 , 0.469999 , 5.71414 , 9.55642 , 11.3824 , 14.0422 ,
23.1052 , 19.9887 , 12.601 , 18.599 , 12.9187 , 17.8309 , 13.4661 , 16.9235 , 16.0927 ,
12.7148 , 12.5723 , 13.1767 , 15.3622 , 12.1449 , 11.9484 , 12.33 , 14.9455 , 11.5331 ,
11.316 , 11.553 , 14.3136 , 13.4346 , 12.8946 , 12.4044};
    double b4[]={2.20159 , 3.56709 , 0.9821 , 168.261 , 10.0953 , 0.542 , 5.1146 ,
0.1403 , 51.6512 , 55.5949 , 0.5826 , 32.9089 , -0.01404 , 26.1476 , 47.3437 , 21.7184
, 129.424 , 14.039 , 7.1937 , 10.1411 , 85.0886 , 8.28524 , 81.6937 , 93.5458 , 6.65365
, 68.1645 , 56.172 , 47.7784 , 60.4486 , 33.3929 , 41.6841 , 31.9128 , 178.437 ,
25.9905 , 51.3531 , 16.0662 , 116.105 , 61.6558 , 15.9768 , 12.9464 , 102.478 , 115.122
, 63.969 , 0.940464 , 98.7399 , 32.4224 , 32.8761 , 83.7543 , 41.3235 , 24.1281 ,
27.573 , 76.8805 , 31.2809 , 38.5566 , 71.1692 , 25.6466 , 18.3491 , 66.3421 , 22.1626
, 16.9673 , 64.8126 , 25.8487 , 19.897 , 58.7097 , 18.0995 , 61.4135 , 14.4122 ,
54.7625 , 11.603 , 47.7972 , 43.8163 , 41.4328 , 58.1535 , 39.3972 , 164.934 , 31.2087
, 132.376 , -0.0138 , 104.354 , -0.01319 , 87.6627 , -0.10276 , 69.7957 , 28.3389 ,
25.7228 , 61.6584 , 26.6307 , 23.3452 , 0 , 86.8472 , 94.2928 , 22.887 , 20.8504 ,
98.6062 , -0.01036 , -0.0102 , 76.8986 , 0 , 0.005127 , 99.8156 , 66.1147 , 0 , 87.4825
, 0 , 92.8029 , 0 , 83.9571 , 62.2061 , -0.7583 , 75.2825 , 55.5113 , 0 , 70.8403 ,
66.8776 , 84.9304 , 64.2658 , 213.904 , 59.4565 , 167.202 , 51.746 , 133.124 , 54.9453
, 127.113 , 43.1692 , 62.2355 , 143.644 , 36.4065 , 45.4643 , 137.903 , 30.8717 ,
132.721 , 27.4491 , 128.007 , 24.8242 , 123.174 , 26.5156 , 22.9966 , 101.398 , 21.7029
, 115.362 , 21.2773 , 111.874 , 19.581 , 92.6566 , 18.5908 , 105.703 , 17.8974 ,
102.961 , 17.2922 , 100.417 , 20.39 , 16.8153 , 84.3298 , 16.3535 , 72.029 , 14.0366 ,
63.3644 , 12.4244 , 57.056 , 11.1972 , 52.0861 , 48.1647 , 18.003 , 45.0011 , 20.3254 ,
17.4911 , 38.6103 , 22.9426 , 16.9392 , 36.3956 , 26.4043 , 18.659 , 38.3246 , 28.2262
, 20.7482 , 45.8149 , 28.8482 , 17.2114 , 47.2579 , 23.8132 , 14.714 , 48.0093 ,
20.3185 , 12.8285 , 47.0045 , 45.4715 , 44.2473 , 150.645 , 142.325 , 29.8436 , 117.02
, 25.9443 , 99.1722 , 23.9533 , 105.251 , 100.613 , 26.3394 , 23.4582 , 25.2017 ,
97.4908 , 25.4928 , 22.7502 , 22.6581 , 105.98 , 24.3992 , 21.8301 , 20.9303 , 102.273
, 88.4834 , 86.003 , 83.7881};
    double c[]={0.001305 , 0.002389 , 0.0064 , 0.0377 , 0.0167 , 0.0385 , -6.1092 ,
-0.1932 , 0.2156 , 0.286977 , -11.529 , 0.2508 , 21.9412 , 0.2776 , 0.653396 , 0.3515 ,

```

```

0.676 , 0.404 , 0.8584 , 0.4853 , 1.1151 , 0.706786 , 1.1407 , 1.24707 , 0.746297 ,
1.1149 , 0.8669 , -9.5574 , -16.378 , 1.4445 , 1.4228 , -4.9978 , 1.3751 , -14.875 ,
1.3329 , -6.6667 , 1.2807 , 0.897155 , -14.652 , -13.28 , 1.2199 , 1.2298 , 0.656565 ,
1.7143 , 1.1832 , 0.616898 , 0.518275 , 1.0896 , 1.0874 , 0.393974 , 0.251877 , 1.0369
, 1.0097 , 0.9707 , 1.0118 , 0.9324 , 0.286667 , 1.0341 , 0.8614 , 0.386044 , 1.191 ,
0.89 , 1.14431 , 1.3041 , 0.7807 , 1.7189 , 1.53545 , 2.1313 , 1.45572 , 2.531 , 2.8409
, 2.9557 , 3.1776 , 2.825 , 3.4873 , 2.0782 , 2.5064 , 41.4025 , 1.91213 , 40.2602 ,
2.06929 , 9.41454 , 3.75591 , -12.912 , -6.3934 , 4.3875 , -14.421 , -14.316 , 0.344941
, 5.40428 , 5.37874 , -3.1892 , 1.42357 , 5.328 , 11.8678 , 11.2835 , 5.26593 , 5.2916
, 13.0174 , 5.179 , 5.21572 , 5.21404 , 5.0694 , 5.11937 , 4.9391 , 4.99635 , 4.7821 ,
4.7861 , 3.9182 , 4.5909 , 4.69626 , 4.69263 , 4.352 , 4.0712 , 4.0714 , 3.7118 ,
3.3352 , 3.2791 , 2.7731 , 3.02902 , 2.14678 , 2.4086 , 1.86264 , 2.09013 , 1.5918 ,
2.0583 , 1.77132 , 1.24285 , 1.98486 , 1.47588 , 2.02876 , 1.19499 , 2.20963 , 0.954586
, 2.5745 , 1.36389 , 0.759344 , 2.4196 , 0.645089 , 3.58324 , 0.691967 , 4.29728 ,
0.68969 , 4.56796 , 0.852795 , 5.92046 , 1.17613 , 6.75621 , 1.63929 , 7.56672 ,
3.70983 , 2.26001 , 7.97628 , 2.97573 , 8.58154 , 2.39699 , 9.24354 , 1.78555 , 9.8875
, 1.01074 , 10.472 , 11.0005 , 6.49804 , 11.4722 , 8.27903 , 6.96824 , 11.6883 ,
9.85329 , 7.39534 , 12.0658 , 11.2299 , 9.0968 , 12.6089 , 12.0205 , 10.6268 , 13.1746
, 12.5258 , 9.8027 , 13.4118 , 12.4734 , 8.08428 , 13.5782 , 12.4711 , -6.7994 , 13.677
, 13.7108 , 13.6905 , 13.7247 , 13.6211 , 13.5431 , 13.5266 , 13.4637 , 13.4314 ,
13.376 , 13.4287 , 13.3966 , 13.3092 , 13.2671 , 13.1665 , 13.3573 , 13.2544 , 13.2116
, 13.113 , 13.3812 , 13.1991 , 13.1555 , 13.0582 , 13.3592 , 13.2887 , 13.2754 ,
13.2674};

```

```

//Search for the input specie in the 'elements' array to start the calculation
for (i=0;i<211;i++){
    if(strcmp(specie, elements[i]) == 0 )
    {
        n=i;
        found = 1;
        break;
    }
}
//If the specie is found in the table
if (found==1){
    //Use the atomic form factor formula which is the sum of the Gaussians
of a particular form
    result=a1[n]*exp(-b1[n]*pow(q/(4*M_PI),2))+a2[n]*exp(-
b2[n]*pow(q/(4*M_PI),2))+a3[n]*exp(-b3[n]*pow(q/(4*M_PI),2))+a4[n]*exp(-
b4[n]*pow(q/(4*M_PI),2))+c[n];
}else{
    //Return error code in case the input specie is not found in the
database
    result=9898989898989898;
}
return result;
}

```

```

/*
The following function takes the value of h,k,l and atomic species array,
as well as the corresponding x,y,z position arrays
and returns the real part of the structure factor for a given value of h,k,l and theta
and lambda
*/

```

```

double realStructFactor(int h, int k, int l, double theta, double lambda, int nat, char
species[nat][10], double x[], double y[], double z[]){

```

```

double result=0;
int i;
double q=4*M_PI*sin(theta)/lambda;
for (i=0;i<nat;i++){
    result=result+formFactorCalc(q,
species[i])*cos(2*M_PI*(h*x[i]+k*y[i]+l*z[i]));
}
return result;
}
/*
The following function takes the value of h,k,l and atomic species array,
as well as the corresponding x,y,z position arrays
and returns the imaginary part of the structure factor for a given value of h,k,l and
theta and lambda.
*/
double imagStructFactor(int h, int k, int l, double theta, double lambda, int nat, char
species[nat][10], double x[], double y[], double z[]){
    double result=0;
    int i;
    double q=4*M_PI*sin(theta)/lambda;
    for (i=0;i<nat;i++){
        result=result+formFactorCalc(q,
species[i])*sin(2*M_PI*(h*x[i]+k*y[i]+l*z[i]));
    }
    return result;
}
main(){
    int nat,h,k,l,i;
    printf("Enter the no. of atoms:\n");
    scanf("%d",&nat);
    double xpos[nat], ypos[nat], zpos[nat];
    char elem[nat][10];
    double theta;
    double lambda;
    printf("Enter the atomic species:\n");
    for(i=0;i<nat;i++){
        scanf("%s",&elem[i]);
    }
    printf("Enter the x-position:\n");
    for(i=0;i<nat;i++){
        scanf("%lf",&xpos[i]);
    }
    printf("Enter the y-position:\n");
    for(i=0;i<nat;i++){
        scanf("%lf",&ypos[i]);
    }
    printf("Enter the z-position:\n");
    for(i=0;i<nat;i++){
        scanf("%lf",&zpos[i]);
    }
    printf("Enter the value of hkl for which the structure factor is required:\n");
    scanf("%d\t%d\t%d",&h,&k,&l);
    printf("Enter the value of theta for which the structure factor is
required:\n");

```

```

scanf("%lf",&theta);
printf("Enter the value of lambda:\n");
scanf("%lf",&lambda);
printf("The real part of structure factor =
%lf\n",realStructFactor(h,k,l,theta,lambda,nat,elem,xpos,ypos,zpos));
printf("The imaginary part of structure factor =
%lf\n",imagStructFactor(h,k,l,theta,lambda,nat,elem,xpos,ypos,zpos));
}

```

Ver. 2 CODE:

```

/*Structure Factor calculator
By: Manas Sharma
mail: feedback@bragitoff.com
http://bragitoff.com
IG: @__physwhiz__ */
#include<stdio.h>
#include<string.h>
#include<math.h>
/*
The following function takes the value of q(scattering vector) in the range 0 to 25
(Angstrom)^-1
and the name of the atomic specie using the atomic symbols
and returns the atomic form factor at that q value.
*/
double formFactorCalc(double q, char specie[]){
    //variable that will store the resulting form factor
    double result;
    int i, found=0,n;
    //Necessary tables needed for the calculations in array form
    char elements[211][10]={"H","H1-
", "He", "Li", "Li1+", "Be", "Be2+", "B", "C", "Cval", "N", "O", "O1-", "F", "F1-
", "Ne", "Na", "Na1+", "Mg", "Mg2+", "Al", "Al3+", "Si", "Si1+", "Si4+", "P", "S", "Cl", "Cl1-
", "Ar", "K", "K1+", "Ca", "Ca2+", "Sc", "Sc3+", "Ti", "Ti2+", "Ti3+", "Ti4+", "V", "V2+", "V3+", "V5+
", "Cr", "Cr2+", "Cr3+", "Mn", "Mn2+", "Mn3+", "Mn4+", "Fe", "Fe2+", "Fe3+", "Co", "Co2+", "Co3+", "N
i", "Ni2+", "Ni3+", "Cu", "Cu1+", "Cu2+", "Zn", "Zn2+", "Ga", "Ga3+", "Ge", "Ge4+", "As", "Se", "Br",
"Br1-
", "Kr", "Rb", "Rb1+", "Sr", "Sr2+", "Y", "Y3+", "Zr", "Zr4+", "Nb", "Nb3+", "Nb5+", "Mo", "Mo3+", "Mo
5+", "Mo6+", "Tc", "Ru", "Ru3+", "Ru4+", "Rh", "Rh3+", "Rh4+", "Pd", "Pd2+", "Pd4+", "Ag", "Ag1+", "A
g2+", "Cd", "Cd2+", "In", "In3+", "Sn", "Sn2+", "Sn4+", "Sb", "Sb3+", "Sb5+", "Te", "I", "I1-
", "Xe", "Cs", "Cs1+", "Ba", "Ba2+", "La", "La3+", "Ce", "Ce3+", "Ce4+", "Pr", "Pr3+", "Pr4+", "Nd", "
Nd3+", "Pm", "Pm3+", "Sm", "Sm3+", "Eu", "Eu2+", "Eu3+", "Gd", "Gd3+", "Tb", "Tb3+", "Dy", "Dy3+", "H
o", "Ho3+", "Er", "Er3+", "Tm", "Tm3+", "Yb", "Yb2+", "Yb3+", "Lu", "Lu3+", "Hf", "Hf4+", "Ta", "Ta5+
", "W", "W6+", "Re", "Os", "Os4+", "Ir", "Ir3+", "Ir4+", "Pt", "Pt2+", "Pt4+", "Au", "Au1+", "Au3+", "
Hg", "Hg1+", "Hg2+", "Tl", "Tl1+", "Tl3+", "Pb", "Pb2+", "Pb4+", "Bi", "Bi3+", "Bi5+", "Po", "At", "R
n", "Fr", "Ra", "Ra2+", "Ac", "Ac3+", "Th", "Th4+", "Pa", "U", "U3+", "U4+", "U6+", "Np", "Np3+", "Np4
+", "Np6+", "Pu", "Pu3+", "Pu4+", "Pu6+", "Am", "Cm", "Bk", "Cf"};
    double a1[]={0.489918 , 0.897661 , 0.8734 , 1.1282 , 0.6968 , 1.5919 , 6.2603 ,
2.0545 , 2.31 , 2.26069 , 12.2126 , 3.0485 , 4.1916 , 3.5392 , 3.6322 , 3.9553 , 4.7626
, 3.2565 , 5.4204 , 3.4988 , 6.4202 , 4.17448 , 6.2915 , 5.66269 , 4.43918 , 6.4345 ,
6.9053 , 11.4604 , 18.2915 , 7.4845 , 8.2186 , 7.9578 , 8.6266 , 15.6348 , 9.189 ,
13.4008 , 9.7595 , 9.11423 , 17.7344 , 19.5114 , 10.2971 , 10.106 , 9.43141 , 15.6887 ,
10.6406 , 9.54034 , 9.6809 , 11.2819 , 10.8061 , 9.84521 , 9.96253 , 11.7695 , 11.0424

```



```
, 11.1764 , 12.2841 , 11.2296 , 10.338 , 12.8376 , 11.4166 , 10.7806 , 13.338 , 11.9475
, 11.8168 , 14.0743 , 11.9719 , 15.2354 , 12.692 , 16.0816 , 12.9172 , 16.6723 ,
17.0006 , 17.1789 , 17.1718 , 17.3555 , 17.1784 , 17.5816 , 17.5663 , 18.0874 , 17.776
, 17.9268 , 17.8765 , 18.1668 , 17.6142 , 19.8812 , 17.9163 , 3.7025 , 21.1664 ,
21.0149 , 17.8871 , 19.1301 , 19.2674 , 18.5638 , 18.5003 , 19.2957 , 18.8785 , 18.8545
, 19.3319 , 19.1701 , 19.2493 , 19.2808 , 19.1812 , 19.1643 , 19.2214 , 19.1514 ,
19.1624 , 19.1045 , 19.1889 , 19.1094 , 18.9333 , 19.6418 , 18.9755 , 19.8685 , 19.9644
, 20.1472 , 20.2332 , 20.2933 , 20.3892 , 20.3524 , 20.3361 , 20.1807 , 20.578 ,
20.2489 , 21.1671 , 20.8036 , 20.3235 , 22.044 , 21.3727 , 20.9413 , 22.6845 , 21.961 ,
23.3405 , 22.5527 , 24.0042 , 23.1504 , 24.6274 , 24.0063 , 23.7497 , 25.0709 , 24.3466
, 25.8976 , 24.9559 , 26.507 , 25.5395 , 26.9049 , 26.1296 , 27.6563 , 26.722 , 28.1819
, 27.3083 , 28.6641 , 28.1209 , 27.8917 , 28.9476 , 28.4628 , 29.144 , 28.8131 ,
29.2024 , 29.1587 , 29.0818 , 29.4936 , 28.7621 , 28.1894 , 30.419 , 27.3049 , 30.4156
, 30.7058 , 27.0059 , 29.8429 , 30.9612 , 16.8819 , 28.0109 , 30.6886 , 20.6809 ,
25.0853 , 29.5641 , 27.5446 , 21.3985 , 30.8695 , 31.0617 , 21.7886 , 32.1244 , 33.3689
, 21.8053 , 33.5364 , 34.6726 , 35.3163 , 35.5631 , 35.9299 , 35.763 , 35.215 , 35.6597
, 35.1736 , 35.5645 , 35.1007 , 35.8847 , 36.0228 , 35.5747 , 35.3715 , 34.8509 ,
36.1874 , 35.7074 , 35.5103 , 35.0136 , 36.5254 , 35.84 , 35.6493 , 35.1736 , 36.6706 ,
36.6488 , 36.7881 , 36.9185};
```

```
double a2[]={0.262003 , 0.565616 , 0.6309 , 0.7508 , 0.7888 , 1.1278 , 0.8849 ,
1.3326 , 1.02 , 1.56165 , 3.1322 , 2.2868 , 1.63969 , 2.6412 , 3.51057 , 3.1125 ,
3.1736 , 3.9362 , 2.1735 , 3.8378 , 1.9002 , 3.3876 , 3.0353 , 3.07164 , 3.20345 ,
4.1791 , 5.2034 , 7.1964 , 7.2084 , 6.7723 , 7.4398 , 7.4917 , 7.3873 , 7.9518 , 7.3679
, 8.0273 , 7.3558 , 7.62174 , 8.73816 , 8.23473 , 7.3511 , 7.3541 , 7.7419 , 8.14208 ,
7.3537 , 7.7509 , 7.81136 , 7.3573 , 7.362 , 7.87194 , 7.97057 , 7.3573 , 7.374 ,
7.3863 , 7.3409 , 7.3883 , 7.88173 , 7.292 , 7.4005 , 7.75868 , 7.1676 , 7.3573 ,
7.11181 , 7.0318 , 7.3862 , 6.7006 , 6.69883 , 6.3747 , 6.70003 , 6.0701 , 5.8196 ,
5.2358 , 6.3338 , 6.7286 , 9.6435 , 7.6598 , 9.8184 , 8.1373 , 10.2946 , 9.1531 ,
10.948 , 10.0562 , 12.0144 , 18.0653 , 13.3417 , 17.2356 , 18.2017 , 18.0992 , 11.175 ,
11.0948 , 12.9182 , 13.2885 , 13.1787 , 14.3501 , 14.1259 , 13.9806 , 15.5017 , 15.2096
, 14.79 , 16.6885 , 15.9719 , 16.2456 , 17.6444 , 17.2535 , 18.5596 , 18.1108 , 19.1005
, 19.0548 , 19.7131 , 19.0455 , 18.933 , 19.0302 , 19.0138 , 18.9949 , 18.997 , 19.0298
, 19.1062 , 19.1278 , 19.297 , 19.1136 , 19.599 , 19.3763 , 19.7695 , 19.559 , 19.8186
, 19.6697 , 19.7491 , 20.0539 , 19.6847 , 19.9339 , 19.6095 , 20.1108 , 19.4258 ,
20.2599 , 19.0886 , 19.9504 , 20.3745 , 19.0798 , 20.4208 , 18.2185 , 20.3271 , 17.6383
, 20.2861 , 17.294 , 20.0994 , 16.4285 , 19.7748 , 15.8851 , 19.332 , 15.4345 , 17.6817
, 18.7614 , 15.2208 , 18.121 , 15.1726 , 18.4601 , 15.2293 , 18.8407 , 15.43 , 19.3763
, 15.7189 , 16.155 , 15.2637 , 16.7296 , 15.862 , 15.5512 , 17.7639 , 16.7224 , 15.9829
, 18.5913 , 17.8204 , 16.9029 , 19.0417 , 18.4973 , 18.06 , 19.1584 , 20.4723 , 18.3481
, 13.0637 , 19.5682 , 18.8003 , 12.951 , 19.5026 , 25.0946 , 15.4733 , 19.0211 ,
21.2816 , 23.0547 , 22.9064 , 21.67 , 23.1032 , 22.1112 , 23.4219 , 22.4418 , 23.2948 ,
23.4128 , 22.5259 , 22.5326 , 22.7584 , 23.5964 , 22.613 , 22.5787 , 22.7286 , 23.8083
, 22.7169 , 22.646 , 22.7181 , 24.0992 , 24.4096 , 24.7736 , 25.1995};
```

```
double a3[]={0.196767 , 0.415815 , 0.3112 , 0.6175 , 0.3414 , 0.5391 , 0.7993 ,
1.0979 , 1.5886 , 1.05075 , 2.0125 , 1.5463 , 1.52673 , 1.517 , 1.26064 , 1.4546 ,
1.2674 , 1.3998 , 1.2269 , 1.3284 , 1.5936 , 1.20296 , 1.9891 , 2.62446 , 1.19453 ,
1.78 , 1.4379 , 6.2556 , 6.5337 , 0.6539 , 1.0519 , 6.359 , 1.5899 , 8.4372 , 1.6409 ,
1.65943 , 1.6991 , 2.2793 , 5.25691 , 2.01341 , 2.0703 , 2.2884 , 2.15343 , 2.03081 ,
3.324 , 3.58274 , 2.87603 , 3.0193 , 3.5268 , 3.56531 , 2.76067 , 3.5222 , 4.1346 ,
3.3948 , 4.0034 , 4.7393 , 4.76795 , 4.4438 , 5.3442 , 5.22746 , 5.6158 , 6.2455 ,
5.78135 , 5.1652 , 6.4668 , 4.3591 , 6.06692 , 3.7068 , 6.06791 , 3.4313 , 3.9731 ,
5.6377 , 5.5754 , 5.5493 , 5.1399 , 5.8981 , 5.422 , 2.5654 , 5.72629 , 1.76795 ,
5.41732 , 1.01118 , 4.04183 , 11.0177 , 10.799 , 12.8876 , 11.7423 , 11.4632 , 6.57891
, 4.64901 , 4.86337 , 9.32602 , 4.71304 , 4.73425 , 3.32515 , 2.53464 , 5.29537 ,
```

```
4.32234 , 2.89289 , 4.8045 , 5.27475 , 4.3709 , 4.461 , 4.47128 , 4.2948 , 3.78897 ,
4.4585 , 4.5648 , 3.4182 , 5.0371 , 5.10789 , 2.41253 , 6.14487 , 7.5138 , 7.8069 ,
8.9767 , 10.662 , 10.2821 , 10.888 , 10.9054 , 11.3727 , 11.6323 , 11.8513 , 11.9369 ,
12.1233 , 12.3856 , 12.1329 , 12.4668 , 12.774 , 12.12 , 13.1235 , 12.0671 , 13.4396 ,
11.9202 , 13.7603 , 11.8034 , 11.8509 , 13.8518 , 11.8708 , 14.3167 , 12.2471 , 14.5596
, 11.9812 , 14.5583 , 11.9788 , 14.9779 , 12.1506 , 15.1542 , 12.3339 , 15.3087 ,
13.3335 , 12.6072 , 15.1 , 12.8429 , 14.7586 , 12.7285 , 14.5135 , 12.8268 , 14.4327 ,
13.0544 , 14.5564 , 14.9305 , 14.7458 , 15.6115 , 13.6145 , 14.2326 , 15.7131 , 13.2153
, 13.7348 , 25.5582 , 14.3359 , 12.7801 , 21.6575 , 16.8883 , 12.8374 , 15.538 ,
18.7478 , 11.9328 , 18.442 , 19.1406 , 12.0175 , 16.5877 , 19.1053 , 19.2497 , 13.1138
, 9.49887 , 8.0037 , 12.1439 , 12.4739 , 7.91342 , 12.5977 , 8.19216 , 12.7473 ,
9.78554 , 14.1891 , 14.9491 , 12.2165 , 12.0291 , 14.0099 , 15.6402 , 12.9898 , 12.7766
, 14.3884 , 16.7707 , 13.5807 , 13.3595 , 14.7635 , 17.3415 , 17.399 , 17.8919 ,
18.3317};
```

```
double a4[]={0.049879 , 0.116973 , 0.178 , 0.4653 , 0.1563 , 0.7029 , 0.1647 ,
0.7068 , 0.865 , 0.839259 , 1.1663 , 0.867 , -20.307 , 1.0243 , 0.940706 , 1.1251 ,
1.1128 , 1.0032 , 2.3073 , 0.8497 , 1.9646 , 0.528137 , 1.541 , 1.3932 , 0.41653 ,
1.4908 , 1.5863 , 1.6455 , 2.3386 , 1.6442 , 0.8659 , 1.1915 , 1.0211 , 0.8537 , 1.468
, 1.57936 , 1.9021 , 0.087899 , 1.92134 , 1.5208 , 2.0571 , 0.0223 , 0.016865 , -9.576
, 1.4922 , 0.509107 , 0.113575 , 2.2441 , 0.2184 , 0.323613 , 0.054447 , 2.3045 ,
0.4399 , 0.0724 , 2.3488 , 0.7108 , 0.725591 , 2.38 , 0.9773 , 0.847114 , 1.6735 ,
1.5578 , 1.14523 , 2.41 , 1.394 , 2.9623 , 1.0066 , 3.683 , 0.859041 , 4.2779 , 4.3543
, 3.9851 , 3.7272 , 3.5375 , 1.5292 , 2.7817 , 2.6694 , -34.193 , 3.26588 , -33.108 ,
3.65721 , -2.6479 , 3.53346 , 1.94715 , 0.337905 , 3.7429 , 2.30951 , 0.740625 , 0 ,
2.71263 , 1.56756 , 3.00964 , 2.18535 , 1.28918 , -6.1989 , -5.6526 , 0.605844 , 0 ,
-7.9492 , 1.0463 , 0.357534 , 0 , 1.6029 , 0 , 2.0396 , 0 , 2.4663 , 0.487 , 0.0193 ,
2.6827 , 0.288753 , 0 , 2.5239 , 2.2735 , 2.8868 , 1.99 , 1.4953 , 0.9615 , 2.6959 ,
0.77634 , 3.28719 , 0.336048 , 3.33049 , 0.612376 , 0.144583 , 2.82428 , 0.97518 ,
0.296689 , 2.85137 , 1.51031 , 2.87516 , 2.07492 , 2.89604 , 2.71488 , 2.9227 , 3.87243
, 3.26503 , 3.54545 , 3.7149 , 2.95354 , 3.773 , 2.96577 , 4.50073 , 3.63837 , 4.93676
, 2.98233 , 5.17379 , 2.98706 , 5.38348 , 2.98963 , 5.14657 , 5.47647 , 3.71601 ,
5.59415 , 4.30013 , 5.59927 , 4.76492 , 5.38695 , 5.11982 , 5.06412 , 5.44174 , 5.67589
, 5.06795 , 5.83377 , 5.82008 , 5.53672 , 5.7837 , 6.35234 , 5.92034 , 5.86 , 6.58077 ,
6.52354 , 5.9676 , 6.48216 , 6.89912 , 5.52593 , 6.82847 , 7.00574 , 5.9696 , 7.01107 ,
6.96886 , 6.4692 , 7.10295 , 6.91555 , 7.02588 , 7.42518 , 7.4433 , 2.11253 , 3.21097 ,
7.65078 , 4.08655 , 7.05545 , 4.80703 , 5.29444 , 4.17287 , 4.188 , 5.37073 , 4.7984 ,
1.21457 , 4.1855 , 5.43227 , 4.92159 , 1.75669 , 3.47947 , 5.66016 , 5.18831 , 2.28678
, 3.49331 , 4.21665 , 4.23284 , 4.24391};
```

```
double b1[]={20.6593 , 53.1368 , 9.1037 , 3.9546 , 4.6237 , 43.6427 , 0.0027 ,
23.2185 , 20.8439 , 22.6907 , 0.0057 , 13.2771 , 12.8573 , 10.2825 , 5.27756 , 8.4042 ,
3.285 , 2.6671 , 2.8275 , 2.1676 , 3.0387 , 1.93816 , 2.4386 , 2.6652 , 1.64167 ,
1.9067 , 1.4679 , 0.0104 , 0.0066 , 0.9072 , 12.7949 , 12.6331 , 10.4421 , -0.0074 ,
9.0213 , 0.29854 , 7.8508 , 7.5243 , 0.22061 , 0.178847 , 6.8657 , 6.8818 , 6.39535 ,
0.679003 , 6.1038 , 5.66078 , 5.59463 , 5.3409 , 5.2796 , 4.91797 , 4.8485 , 4.7611 ,
4.6538 , 4.6147 , 4.2791 , 4.1231 , 3.90969 , 3.8785 , 3.6766 , 3.5477 , 3.5828 ,
3.3669 , 3.37484 , 3.2655 , 2.9946 , 3.0669 , 2.81262 , 2.8509 , 2.53718 , 2.6345 ,
2.4098 , 2.1723 , 2.2059 , 1.9384 , 1.7888 , 1.7139 , 1.5564 , 1.4907 , 1.4029 ,
1.35417 , 1.27618 , 1.2148 , 1.18865 , 0.019175 , 1.12446 , 0.2772 , 0.014734 ,
0.014345 , 1.03649 , 0.864132 , 0.80852 , 0.847329 , 0.844582 , 0.751536 , 0.764252 ,
0.760825 , 0.698655 , 0.696219 , 0.683839 , 0.6446 , 0.646179 , 0.645643 , 0.5946 ,
0.597922 , 0.5476 , 0.551522 , 5.8303 , 0.5036 , 5.764 , 5.3034 , 0.467196 , 5.44853 ,
4.81742 , 4.347 , 4.3579 , 3.9282 , 3.569 , 3.552 , 3.216 , 3.21367 , 2.94817 , 2.9207
, 2.81219 , 2.77691 , 2.65941 , 2.77393 , 2.6452 , 2.54467 , 2.66248 , 2.52722 , 2.5627
, 2.4174 , 2.47274 , 2.31641 , 2.3879 , 2.27783 , 2.22258 , 2.25341 , 2.13553 , 2.24256
```

```
, 2.05601 , 2.1802 , 1.9804 , 2.07051 , 1.91072 , 2.07356 , 1.84659 , 2.02859 , 1.78711
, 1.9889 , 1.78503 , 1.73272 , 1.90182 , 1.68216 , 1.83262 , 1.59136 , 1.77333 ,
1.50711 , 1.72029 , 1.42755 , 1.67191 , 1.62903 , 1.37113 , 1.59279 , 1.34323 , 1.30923
, 1.51293 , 1.32927 , 1.24813 , 0.4611 , 1.35321 , 1.2199 , 0.545 , 1.39507 , 1.21152 ,
0.65515 , 1.4711 , 1.1008 , 0.6902 , 1.3366 , 1.00566 , 0.704 , 1.2356 , 0.91654 ,
0.700999 , 0.68587 , 0.6631 , 0.646453 , 0.616341 , 0.604909 , 0.589092 , 0.579689 ,
0.563359 , 0.555054 , 0.547751 , 0.5293 , 0.52048 , 0.516598 , 0.507079 , 0.511929 ,
0.502322 , 0.498626 , 0.48981 , 0.499384 , 0.484938 , 0.481422 , 0.473204 , 0.483629 ,
0.465154 , 0.451018 , 0.437533};
```

```
double b2[]={7.74039 , 15.187 , 3.3568 , 1.0524 , 1.9557 , 1.8623 , 0.8313 ,
1.021 , 10.2075 , 0.656665 , 9.8933 , 5.7011 , 4.17236 , 4.2944 , 14.7353 , 3.4262 ,
8.8422 , 6.1153 , 79.2611 , 4.7542 , 0.7426 , 4.14553 , 32.3337 , 38.6634 , 3.43757 ,
27.157 , 22.2151 , 1.1662 , 1.1717 , 14.8407 , 0.7748 , 0.7674 , 0.6599 , 0.6089 ,
0.5729 , 7.9629 , 0.5 , 0.457585 , 7.04716 , 6.67018 , 0.4385 , 0.4409 , 0.383349 ,
5.40135 , 0.392 , 0.344261 , 0.334393 , 0.3432 , 0.3435 , 0.294393 , 0.283303 , 0.3072
, 0.3053 , 0.3005 , 0.2784 , 0.2726 , 0.238668 , 0.2565 , 0.2449 , 0.22314 , 0.247 ,
0.2274 , 0.244078 , 0.2333 , 0.2031 , 0.2412 , 0.22789 , 0.2516 , 0.205855 , 0.2647 ,
0.2726 , 16.5796 , 19.3345 , 16.5623 , 17.3151 , 14.7957 , 14.0988 , 12.6963 , 12.8006
, 11.2145 , 11.916 , 10.1483 , 11.766 , 1.13305 , 0.028781 , 1.0958 , 1.03031 , 1.02238
, 8.48061 , 8.14487 , 8.43467 , 8.37164 , 8.12534 , 8.21758 , 7.84438 , 7.62436 ,
7.98929 , 7.55573 , 7.14833 , 7.4726 , 7.19123 , 7.18544 , 6.9089 , 6.80639 , 6.3776 ,
6.3247 , 0.5031 , 5.8378 , 0.4655 , 0.4607 , 5.22126 , 0.467973 , 0.420885 , 0.3814 ,
0.3815 , 0.344 , 0.3107 , 0.3086 , 0.2756 , 0.28331 , 0.244475 , 0.250698 , 0.226836 ,
0.23154 , 0.21885 , 0.222087 , 0.214299 , 0.202481 , 0.210628 , 0.199237 , 0.202088 ,
0.185769 , 0.196451 , 0.174081 , 0.1942 , 0.17353 , 0.16394 , 0.181951 , 0.155525 ,
0.196143 , 0.149525 , 0.202172 , 0.143384 , 0.19794 , 0.139358 , 0.223545 , 0.13729 ,
0.238849 , 0.136974 , 0.257119 , 0.15997 , 0.13879 , 9.98519 , 0.142292 , 9.5999 ,
0.128903 , 9.37046 , 0.116741 , 9.2259 , 0.104621 , 9.09227 , 8.97948 , 6.84706 ,
8.86553 , 7.10909 , 6.71983 , 8.81174 , 7.38979 , 6.60834 , 8.6216 , 7.7395 , 6.82872 ,
8.4484 , 7.65105 , 7.05639 , 8.70751 , 0.517394 , 6.53852 , 2.3576 , 0.488383 , 6.10926
, 2.9238 , 6.24149 , 0.39042 , 3.55078 , 3.97458 , 4.0691 , 4.17619 , 3.87135 , 3.5767
, 3.65155 , 3.41437 , 3.46204 , 3.24498 , 3.41519 , 3.3253 , 3.12293 , 3.05053 , 2.8903
, 3.25396 , 3.03807 , 2.96627 , 2.81099 , 3.26371 , 2.96118 , 2.8902 , 2.73848 ,
3.20647 , 3.08997 , 3.04619 , 3.00775};
```

```
double b3[]={49.5519 , 186.576 , 22.9276 , 85.3905 , 0.6316 , 103.483 , 2.2758
, 60.3498 , 0.5687 , 9.75618 , 28.9975 , 0.3239 , 47.0179 , 0.2615 , 0.442258 , 0.2306
, 0.3136 , 0.2001 , 0.3808 , 0.185 , 31.5472 , 0.228753 , 0.6785 , 0.916946 , 0.2149 ,
0.526 , 0.2536 , 18.5194 , 19.5424 , 43.8983 , 213.187 , -0.002 , 85.7484 , 10.3116 ,
136.108 , -0.28604 , 35.6338 , 19.5361 , -0.15762 , -0.29263 , 26.8938 , 20.3004 ,
15.1908 , 9.97278 , 20.2626 , 13.3075 , 12.8288 , 17.8674 , 14.343 , 10.8171 , 10.4852
, 15.3535 , 12.0546 , 11.6729 , 13.5359 , 10.2443 , 8.35583 , 12.1763 , 8.873 , 7.64468
, 11.3966 , 8.6625 , 7.9876 , 10.3163 , 7.0826 , 10.7805 , 6.36441 , 11.4468 , 5.47913
, 12.9479 , 15.2372 , 0.2609 , 0.2871 , 0.2261 , 0.2748 , 0.1603 , 0.1664 , 24.5651 ,
0.125599 , 22.6599 , 0.117622 , 21.6054 , 0.204785 , 10.1621 , 9.28206 , 11.004 ,
9.53659 , 8.78809 , 0.058881 , 21.5707 , 24.7997 , 0.017662 , 0.36495 , 25.8749 ,
21.2487 , 19.3317 , 25.2052 , 22.5057 , 17.9144 , 24.6605 , 21.7326 , 21.4072 , 24.7008
, 20.2521 , 25.8499 , 17.3595 , 26.8909 , 23.3752 , 14.0049 , 27.9074 , 19.5902 ,
14.1259 , 28.5284 , 27.766 , 29.5259 , 26.4659 , 24.3879 , 23.7128 , 20.2073 , 20.0558
, 18.7726 , 17.8211 , 17.6083 , 16.5408 , 15.7992 , 16.7669 , 15.323 , 14.8137 , 15.885
, 14.1783 , 15.1009 , 13.1275 , 14.3996 , 12.1571 , 13.7546 , 11.6096 , 11.311 ,
12.9331 , 10.5782 , 12.6648 , 10.0499 , 12.1899 , 9.34972 , 11.4407 , 8.80018 , 11.3604
, 8.36225 , 10.9975 , 7.96778 , 10.6647 , 8.18304 , 7.64412 , 0.261033 , 7.33727 ,
0.275116 , 6.76232 , 0.295977 , 6.31524 , 0.321703 , 5.93667 , 0.3505 , 0.382661 ,
0.165191 , 0.417916 , 0.204633 , 0.167252 , 0.424593 , 0.263297 , 0.16864 , 1.4826 ,
```

```

0.356752 , 0.212867 , 1.5729 , 0.443378 , 0.284738 , 1.96347 , 7.43463 , 0.219074 ,
8.618 , 6.7727 , 0.147041 , 8.7937 , 0.469999 , 5.71414 , 9.55642 , 11.3824 , 14.0422 ,
23.1052 , 19.9887 , 12.601 , 18.599 , 12.9187 , 17.8309 , 13.4661 , 16.9235 , 16.0927 ,
12.7148 , 12.5723 , 13.1767 , 15.3622 , 12.1449 , 11.9484 , 12.33 , 14.9455 , 11.5331 ,
11.316 , 11.553 , 14.3136 , 13.4346 , 12.8946 , 12.4044};
    double b4[]={2.20159 , 3.56709 , 0.9821 , 168.261 , 10.0953 , 0.542 , 5.1146 ,
0.1403 , 51.6512 , 55.5949 , 0.5826 , 32.9089 , -0.01404 , 26.1476 , 47.3437 , 21.7184
, 129.424 , 14.039 , 7.1937 , 10.1411 , 85.0886 , 8.28524 , 81.6937 , 93.5458 , 6.65365
, 68.1645 , 56.172 , 47.7784 , 60.4486 , 33.3929 , 41.6841 , 31.9128 , 178.437 ,
25.9905 , 51.3531 , 16.0662 , 116.105 , 61.6558 , 15.9768 , 12.9464 , 102.478 , 115.122
, 63.969 , 0.940464 , 98.7399 , 32.4224 , 32.8761 , 83.7543 , 41.3235 , 24.1281 ,
27.573 , 76.8805 , 31.2809 , 38.5566 , 71.1692 , 25.6466 , 18.3491 , 66.3421 , 22.1626
, 16.9673 , 64.8126 , 25.8487 , 19.897 , 58.7097 , 18.0995 , 61.4135 , 14.4122 ,
54.7625 , 11.603 , 47.7972 , 43.8163 , 41.4328 , 58.1535 , 39.3972 , 164.934 , 31.2087
, 132.376 , -0.0138 , 104.354 , -0.01319 , 87.6627 , -0.10276 , 69.7957 , 28.3389 ,
25.7228 , 61.6584 , 26.6307 , 23.3452 , 0 , 86.8472 , 94.2928 , 22.887 , 20.8504 ,
98.6062 , -0.01036 , -0.0102 , 76.8986 , 0 , 0.005127 , 99.8156 , 66.1147 , 0 , 87.4825
, 0 , 92.8029 , 0 , 83.9571 , 62.2061 , -0.7583 , 75.2825 , 55.5113 , 0 , 70.8403 ,
66.8776 , 84.9304 , 64.2658 , 213.904 , 59.4565 , 167.202 , 51.746 , 133.124 , 54.9453
, 127.113 , 43.1692 , 62.2355 , 143.644 , 36.4065 , 45.4643 , 137.903 , 30.8717 ,
132.721 , 27.4491 , 128.007 , 24.8242 , 123.174 , 26.5156 , 22.9966 , 101.398 , 21.7029
, 115.362 , 21.2773 , 111.874 , 19.581 , 92.6566 , 18.5908 , 105.703 , 17.8974 ,
102.961 , 17.2922 , 100.417 , 20.39 , 16.8153 , 84.3298 , 16.3535 , 72.029 , 14.0366 ,
63.3644 , 12.4244 , 57.056 , 11.1972 , 52.0861 , 48.1647 , 18.003 , 45.0011 , 20.3254 ,
17.4911 , 38.6103 , 22.9426 , 16.9392 , 36.3956 , 26.4043 , 18.659 , 38.3246 , 28.2262
, 20.7482 , 45.8149 , 28.8482 , 17.2114 , 47.2579 , 23.8132 , 14.714 , 48.0093 ,
20.3185 , 12.8285 , 47.0045 , 45.4715 , 44.2473 , 150.645 , 142.325 , 29.8436 , 117.02
, 25.9443 , 99.1722 , 23.9533 , 105.251 , 100.613 , 26.3394 , 23.4582 , 25.2017 ,
97.4908 , 25.4928 , 22.7502 , 22.6581 , 105.98 , 24.3992 , 21.8301 , 20.9303 , 102.273
, 88.4834 , 86.003 , 83.7881};
    double c[]={0.001305 , 0.002389 , 0.0064 , 0.0377 , 0.0167 , 0.0385 , -6.1092 ,
-0.1932 , 0.2156 , 0.286977 , -11.529 , 0.2508 , 21.9412 , 0.2776 , 0.653396 , 0.3515 ,
0.676 , 0.404 , 0.8584 , 0.4853 , 1.1151 , 0.706786 , 1.1407 , 1.24707 , 0.746297 ,
1.1149 , 0.8669 , -9.5574 , -16.378 , 1.4445 , 1.4228 , -4.9978 , 1.3751 , -14.875 ,
1.3329 , -6.6667 , 1.2807 , 0.897155 , -14.652 , -13.28 , 1.2199 , 1.2298 , 0.656565 ,
1.7143 , 1.1832 , 0.616898 , 0.518275 , 1.0896 , 1.0874 , 0.393974 , 0.251877 , 1.0369
, 1.0097 , 0.9707 , 1.0118 , 0.9324 , 0.286667 , 1.0341 , 0.8614 , 0.386044 , 1.191 ,
0.89 , 1.14431 , 1.3041 , 0.7807 , 1.7189 , 1.53545 , 2.1313 , 1.45572 , 2.531 , 2.8409
, 2.9557 , 3.1776 , 2.825 , 3.4873 , 2.0782 , 2.5064 , 41.4025 , 1.91213 , 40.2602 ,
2.06929 , 9.41454 , 3.75591 , -12.912 , -6.3934 , 4.3875 , -14.421 , -14.316 , 0.344941
, 5.40428 , 5.37874 , -3.1892 , 1.42357 , 5.328 , 11.8678 , 11.2835 , 5.26593 , 5.2916
, 13.0174 , 5.179 , 5.21572 , 5.21404 , 5.0694 , 5.11937 , 4.9391 , 4.99635 , 4.7821 ,
4.7861 , 3.9182 , 4.5909 , 4.69626 , 4.69263 , 4.352 , 4.0712 , 4.0714 , 3.7118 ,
3.3352 , 3.2791 , 2.7731 , 3.02902 , 2.14678 , 2.4086 , 1.86264 , 2.09013 , 1.5918 ,
2.0583 , 1.77132 , 1.24285 , 1.98486 , 1.47588 , 2.02876 , 1.19499 , 2.20963 , 0.954586
, 2.5745 , 1.36389 , 0.759344 , 2.4196 , 0.645089 , 3.58324 , 0.691967 , 4.29728 ,
0.68969 , 4.56796 , 0.852795 , 5.92046 , 1.17613 , 6.75621 , 1.63929 , 7.56672 ,
3.70983 , 2.26001 , 7.97628 , 2.97573 , 8.58154 , 2.39699 , 9.24354 , 1.78555 , 9.8875
, 1.01074 , 10.472 , 11.0005 , 6.49804 , 11.4722 , 8.27903 , 6.96824 , 11.6883 ,
9.85329 , 7.39534 , 12.0658 , 11.2299 , 9.0968 , 12.6089 , 12.0205 , 10.6268 , 13.1746
, 12.5258 , 9.8027 , 13.4118 , 12.4734 , 8.08428 , 13.5782 , 12.4711 , -6.7994 , 13.677
, 13.7108 , 13.6905 , 13.7247 , 13.6211 , 13.5431 , 13.5266 , 13.4637 , 13.4314 ,
13.376 , 13.4287 , 13.3966 , 13.3092 , 13.2671 , 13.1665 , 13.3573 , 13.2544 , 13.2116
, 13.113 , 13.3812 , 13.1991 , 13.1555 , 13.0582 , 13.3592 , 13.2887 , 13.2754 ,

```

```

13.2674};
//Search for the input specie in the 'elements' array to start the calculation
for (i=0;i<211;i++){
    if(strcmp(specie, elements[i]) == 0 )
    {
        n=i;
        found = 1;
        break;
    }
}
//If the specie is found in the table
if (found==1){
    //Use the atomic form factor formula which is the sum of the Gaussians
of a particular form
    result=a1[n]*exp(-b1[n]*pow(q/(4*M_PI),2))+a2[n]*exp(-
b2[n]*pow(q/(4*M_PI),2))+a3[n]*exp(-b3[n]*pow(q/(4*M_PI),2))+a4[n]*exp(-
b4[n]*pow(q/(4*M_PI),2))+c[n];
}else{
    //Return error code in case the input specie is not found in the
database
    result=9898989898989898;
}
return result;
}
/*
The following function takes the value of h,k,l and atomic species array,
as well as the corresponding x,y,z position arrays
and returns the real part of the structure factor for a given value of h,k,l and theta
and lambda
*/
double realStructFactor(int h, int k, int l, double theta, double lambda, int nat, char
species[nat][10], double x[], double y[], double z[]){
    double result=0;
    int i;
    double q=4*M_PI*sin(theta*M_PI/180.0)/lambda;
    for (i=0;i<nat;i++){
        result=result+formFactorCalc(q,
species[i])*cos(2*M_PI*(h*x[i]+k*y[i]+l*z[i]));
    }
    return result;
}
/*
The following function takes the value of h,k,l and atomic species array,
as well as the corresponding x,y,z position arrays
and returns the imaginary part of the structure factor for a given value of h,k,l and
theta and lambda.
*/
double imagStructFactor(int h, int k, int l, double theta, double lambda, int nat, char
species[nat][10], double x[], double y[], double z[]){
    double result=0;
    int i;
    double q=4*M_PI*sin(theta*M_PI/180.0)/lambda;
    for (i=0;i<nat;i++){
        result=result+formFactorCalc(q,

```

```

species[i])*sin(2*M_PI*(h*x[i]+k*y[i]+l*z[i]));
    }
    return result;
}
main(){
    int nat,h,k,l,i;
    FILE *fp=NULL;
    fp=fopen("atomicPos.txt","r");
    //Read the first line that contains the number of atoms
    fscanf(fp,"%d\n",&nat);
    double xpos[nat], ypos[nat], zpos[nat];
    char elem[nat][10];
    double theta;
    double lambda;
    //Skip the second line fo the file
    fscanf(fp,"%*[\n]");
    //Start reading the atom symbol and the x,y,z coordinates
    for(i=0;i<nat;i++){
        fscanf(fp,"%s\t%lf\t%lf\t%lf\n",&elem[i],&xpos[i],&ypos[i],&zpos[i]);
    }
    printf("Enter the value of hkl for which the structure factor is required:\n");
    scanf("%d\t%d\t%d",&h,&k,&l);
    printf("Enter the value of theta for which the structure factor is
required:\n");
    scanf("%lf",&theta);
    printf("Enter the value of lambda:\n");
    scanf("%lf",&lambda);
    printf("The real part of structure factor =
%lf\n",realStructFactor(h,k,l,theta,lambda,nat,elem,xpos,ypos,zpos));
    printf("The imaginary part of structure factor =
%lf\n",imagStructFactor(h,k,l,theta,lambda,nat,elem,xpos,ypos,zpos));
}

```

Input File format:

The input file has to be of a very specific format.

The first line should contain only the number of atoms (Nothing else). The second line is skipped by the code so it can be used to divide the next part using any comment you want. From third line onwards, you can specify the atom species and their coordinates (crystal/fractional coordinates only). They should follow the following order:

```

ATOMIC_POSITIONS {crystal}
Fe 0.00 0.00 0.00
Fe 0.50 0.50 0.50

```

(Make sure the coordinates aren't in the second line as that is skipped)

Overall the file would look like this:

```

8
ATOMIC_POSITIONS {crystal}
Ge 0.000000 0.000000 0.000000
Ge 0.000000 0.500000 0.500000
Ge 0.500000 0.000000 0.500000
Ge 0.500000 0.500000 0.000000
Ge 0.750000 0.750000 0.250000

```

```
Ge 0.750000 0.250000 0.750000
Ge 0.250000 0.750000 0.750000
Ge 0.250000 0.250000 0.250000
```

OUTPUT:

```
manas@ubuntu:~/XRD Simulator$ ./a.out
Enter the no. of atoms:
2
Enter the atomic species:
Fe
Fe
Enter the x-position:
0 0.5
Enter the y-position:
0 0.5
Enter the z-position:
0 0.5
Enter the value of hkl for which the structure factor is required:
1 1 1
Enter the value of theta for which the structure factor is required:
40
Enter the value of lambda:
1.5409
The real part of structure factor = 0.000000
The imaginary part of structure factor = 0.000000
manas@ubuntu:~/XRD Simulator$
```

References:

<http://pd.chem.ucl.ac.uk/pdmn/diff2/structf.htm>

https://en.wikipedia.org/wiki/Structure_factor



[Manas Sharma](#)

I'm a physicist specializing in theoretical, computational and experimental condensed matter physics. I like to develop Physics related apps and softwares from time to time. Can code in most of the popular languages. Like to share my knowledge in Physics and applications using this Blog and a YouTube channel.

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