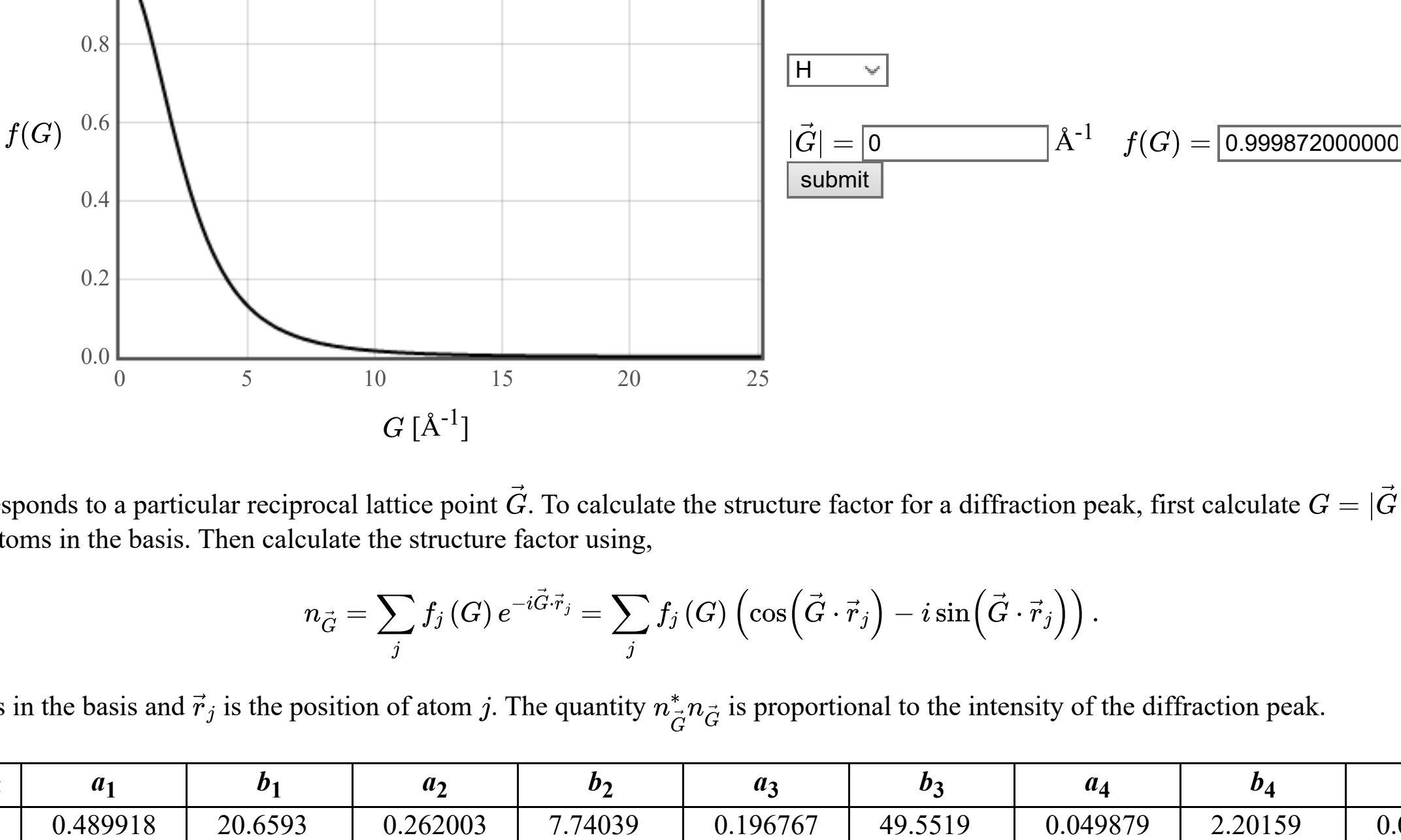


Atomic form factors

The atomic form factor is the Fourier transform of the electron density of an atom. It is assumed that the electron density is spherically symmetric so that the value of the Fourier transform only depends on the distance from the origin in reciprocal space. The diffraction condition is  $\Delta \mathbf{k} = \vec{q} = \vec{G}$  where  $\vec{q}$  is called the scattering vector. In the range of scattering vectors between  $0 < q < 25 \text{ \AA}^{-1}$ , the atomic form factor is well approximated by a sum of Gaussians of the form, [1]

$$f(|\vec{G}|) = \sum_{i=1}^4 a_i \exp\left(-b_i \left(\frac{G}{4\pi}\right)^2\right) + c,$$

where the values of  $a_i$ ,  $b_i$ , and  $c$  are tabulated below. The different atomic form factors for the elements can be plotted using the form below.



Each diffraction peak corresponds to a particular reciprocal lattice point  $\vec{G}$ . To calculate the structure factor for a diffraction peak, first calculate  $G = |\vec{G}|$  and use the form above to calculate  $f(G)$  for all the atoms in the basis. Then calculate the structure factor using,

$$n_{\vec{G}} = \sum_j f_j(G) e^{-i\vec{G} \cdot \vec{r}_j} = \sum_j f_j(G) \left( \cos\left(\vec{G} \cdot \vec{r}_j\right) - i \sin\left(\vec{G} \cdot \vec{r}_j\right) \right).$$

Here  $j$  sums over the atoms in the basis and  $\vec{r}_j$  is the position of atom  $j$ . The quantity  $n_{\vec{G}}^* n_{-\vec{G}}$  is proportional to the intensity of the diffraction peak.

|       |           |          |         |          |         |          |          |          |          |
|-------|-----------|----------|---------|----------|---------|----------|----------|----------|----------|
|       | 4.1916    | 12.8573  | 1.63969 | 4.17236  | 1.52673 | 47.0179  | -20.307  | -0.01404 | 21.9412  |
| F1-   | 3.6322    | 5.27756  | 3.51057 | 14.7353  | 1.26064 | 0.442258 | 0.940706 | 47.3437  | 0.653396 |
| Ne    | 3.9553    | 8.4042   | 3.1125  | 3.4262   | 1.4546  | 0.2306   | 1.1251   | 21.7184  | 0.3515   |
| Na    | 4.7626    | 3.285    | 3.1736  | 8.8422   | 1.2674  | 0.3136   | 1.1128   | 129.424  | 0.676    |
| Na1+  | 3.2565    | 2.6671   | 3.9362  | 6.1153   | 1.3998  | 0.2001   | 1.0032   | 14.039   | 0.404    |
| Mg    | 5.4204    | 2.8275   | 2.1735  | 79.2611  | 1.2269  | 0.3808   | 2.3073   | 7.1937   | 0.8584   |
| Mg2+  | 3.4988    | 2.1676   | 3.8378  | 4.7542   | 1.3284  | 0.185    | 0.8497   | 10.1411  | 0.4853   |
| Al    | 6.4202    | 3.0387   | 1.9002  | 0.7426   | 1.5936  | 31.5472  | 1.9646   | 85.0886  | 1.1151   |
| Al3+  | 4.17448   | 1.93816  | 3.3876  | 4.14553  | 1.20296 | 0.228753 | 0.528137 | 8.28524  | 0.706786 |
| Siv   | 6.2915    | 2.4386   | 3.0353  | 32.3337  | 1.9891  | 0.6785   | 1.541    | 81.6937  | 1.1407   |
| Sival | 5.66269   | 2.6652   | 3.07164 | 38.6634  | 2.62446 | 0.916946 | 1.3932   | 93.5458  | 1.24707  |
| Si4+  | 4.43918   | 1.64167  | 3.20345 | 3.43757  | 1.19453 | 0.2149   | 0.41653  | 6.65365  | 0.746297 |
| P     | 6.4345    | 1.9067   | 4.1791  | 27.157   | 1.78    | 0.526    | 1.4908   | 68.1645  | 1.1149   |
| S     | 6.9053    | 1.4679   | 5.2034  | 22.2151  | 1.4379  | 0.2536   | 1.5863   | 56.172   | 0.8669   |
| Cl    | 11.4604   | 0.0104   | 7.1964  | 1.1662   | 6.2556  | 18.5194  | 1.6455   | 47.7784  | -9.5574  |
| Cl1-  | 18.2915   | 0.0066   | 7.2084  | 1.1717   | 6.5337  | 19.5424  | 2.3386   | 60.4486  | -16.378  |
| Ar    | 7.4845    | 0.9072   | 6.7723  | 14.8407  | 0.6539  | 43.8983  | 1.6442   | 33.3929  | 1.4445   |
| K     | 8.2186    | 12.7949  | 7.4398  | 0.7748   | 1.0519  | 213.187  | 0.8659   | 41.6841  | 1.4228   |
| K1+   | 7.9578    | 12.6331  | 7.4917  | 0.7674   | 6.359   | -0.002   | 1.1915   | 31.9128  | -4.9978  |
| Ca    | 8.6266    | 10.4421  | 7.3873  | 0.6599   | 1.5899  | 85.7484  | 1.0211   | 178.437  | 1.3751   |
| Ca2+  | 15.6348   | -0.0074  | 7.9518  | 0.6089   | 8.4372  | 10.3116  | 0.8537   | 25.9905  | -14.875  |
| Sc    | 9.189     | 9.0213   | 7.3679  | 0.5729   | 1.6409  | 136.108  | 1.468    | 51.3531  | 1.3329   |
| Sc3+  | 13.4008   | 0.29854  | 8.0273  | 7.9629   | 1.65943 | -0.28604 | 1.57936  | 16.0662  | -6.6667  |
| Ti    | 9.7595    | 7.8508   | 7.3558  | 0.5      | 1.6991  | 35.6338  | 1.9021   | 116.105  | 1.2807   |
| Ti2+  | 9.11423   | 7.5243   | 7.62174 | 0.457585 | 2.2793  | 19.5361  | 0.087899 | 61.6558  | 0.897155 |
| Ti3+  | 17.7344   | 0.22061  | 8.73816 | 7.04716  | 5.25691 | -0.15762 | 1.92134  | 15.9768  | -14.652  |
| Ti4+  | 19.5114   | 0.178847 | 8.23473 | 6.67018  | 2.01341 | -0.29263 | 1.5208   | 12.9464  | -13.28   |
| V     | 10.2971   | 6.8657   | 7.3511  | 0.4385   | 2.0703  | 26.8938  | 2.0571   | 102.478  | 1.2199   |
| V2+   | 10.106    | 6.8818   | 7.3541  | 0.4409   | 2.2884  | 20.3004  | 0.0223   | 115.122  | 1.2298   |
| V3+   | 9.43141   | 6.39535  | 7.7419  | 0.383349 | 2.15343 | 15.1908  | 0.016865 | 63.969   | 0.656565 |
| V5+   | 15.6887   | 0.679003 | 8.14208 | 5.40135  | 2.03081 | 9.97278  | -9.576   | 0.940464 | 1.7143   |
| Cr    | 10.6406   | 6.1038   | 7.3537  | 0.392    | 3.324   | 20.2626  | 1.4922   | 98.7399  | 1.1832   |
| Cr2+  | 9.54034   | 5.66078  | 7.7509  | 0.344261 | 3.58274 | 13.3075  | 0.509107 | 32.4224  | 0.616898 |
| Cr3+  | 9.6809    | 5.59463  | 7.81136 | 0.334393 | 2.87603 | 12.8288  | 0.113575 | 32.8761  | 0.518275 |
| Mn    | 11.2819   | 5.3409   | 7.3573  | 0.3432   | 3.0193  | 17.8674  | 2.2441   | 83.7543  | 1.0896   |
| Mn2+  | 10.8061   | 5.2796   | 7.362   | 0.3435   | 3.5268  | 14.343   | 0.2184   | 41.3235  | 1.0874   |
| Mn3+  | 9.84521   | 4.91797  | 7.87194 | 0.294393 | 3.56531 | 10.8171  | 0.323613 | 24.1281  | 0.393974 |
| Mn4+  | 9.96253   | 4.8485   | 7.97057 | 0.283303 | 2.76067 | 10.4852  | 0.054447 | 27.573   | 0.251877 |
| Fe    | 11.7695   | 4.7611   | 7.3573  | 0.3072   | 3.5222  | 15.3535  | 2.3045   | 76.8805  | 1.0369   |
| Fe2+  | 11.0424   | 4.6538   | 7.374   | 0.3053   | 4.1346  | 12.0546  | 0.4399   | 31.2809  | 1.0097   |
| Fe3+  | 11.1764   | 4.6147   | 7.3863  | 0.3005   | 3.3948  | 11.6729  | 0.0724   | 38.5566  | 0.9707   |
| Co    | 12.2841   | 4.2791   | 7.3409  | 0.2784   | 4.0034  | 13.5359  | 2.3488   | 71.1692  | 1.0118   |
| Co2+  | 11.2296   | 4.1231   | 7.3883  | 0.2726   | 4.7393  | 10.2443  | 0.7108   | 25.6466  | 0.9324   |
| Co3+  | 10.338    | 3.90969  | 7.88173 | 0.238668 | 4.76795 | 8.35583  | 0.725591 | 18.3491  | 0.286667 |
| Ni    | 12.8376   | 3.8785   | 7.292   | 0.2565   | 4.4438  | 12.1763  | 2.38     | 66.3421  | 1.0341   |
| Ni2+  | 11.4166   | 3.6766   | 7.4005  | 0.2449   | 5.3442  | 8.873    | 0.9773   | 22.1626  | 0.8614   |
| Ni3+  | 10.7806   | 3.5477   | 7.75868 | 0.22314  | 5.22746 | 7.64468  | 0.847114 | 16.9673  | 0.386044 |
| Cu    | 13.338    | 3.5828   | 7.1676  | 0.247    | 5.6158  | 11.3966  | 1.6735   | 64.8126  | 1.191    |
| Cu1+  | 11.9475   | 3.3669   | 7.3573  | 0.2274   | 6.2455  | 8.6625   | 1.5578   | 25.8487  | 0.89     |
| Cu2+  | 11.8168   | 3.37484  | 7.11181 | 0.244078 | 5.78135 | 7.9876   | 1.14523  | 19.897   | 1.14431  |
| Zn    | 14.0743   | 3.2655   | 7.0318  | 0.2333   | 5.1652  | 10.3163  | 2.41     | 58.7097  | 1.3041   |
| Zn2+  | 11.9719   | 2.9946   | 7.3862  | 0.2031   | 6.4668  | 7.0826   | 1.394    | 18.0995  | 0.7807   |
| Ga    | 15.2354   | 3.0669   | 6.7006  | 0.2412   | 4.3591  | 10.7805  | 2.9623   | 61.4135  | 1.7189   |
| Ga3+  | 12.692    | 2.81262  | 6.69883 | 0.22789  | 6.06692 | 6.36441  | 1.0066   | 14.4122  | 1.53545  |
| Ge    | 16.0816   | 2.8509   | 6.3747  | 0.2516   | 3.7068  | 11.4468  | 3.683    | 54.7625  | 2.1313   |
| Ge4+  | 12.9172   | 2.53718  | 6.70003 | 0.205855 | 6.06791 | 5.47913  | 0.859041 | 11.603   | 1.45572  |
| As    | 16.6723   | 2.6345   | 6.0701  | 0.2647   | 3.4313  | 12.9479  | 4.2779   | 47.7972  | 2.531    |
| Se    | 17.0006   | 2.4098   | 5.8196  | 0.2726   | 3.9731  | 15.2372  | 4.3543   | 43.8163  | 2.8409   |
| Br    | 17.1789   | 2.1723   | 5.2358  | 16.5796  | 5.6377  | 0.2609   | 3.9851   | 41.4328  | 2.9557   |
| Br1-  | 17.1718   | 2.2059   | 6.3338  | 19.3345  | 5.5754  | 0.2871   | 3.7272   | 58.1535  | 3.1776   |
| Kr    | 17.3555   | 1.9384   | 6.7286  | 16.5623  | 5.5493  | 0.2261   | 3.5375   | 39.3972  | 2.825    |
| Rb    | 17.1784   | 1.7888   | 9.6435  | 17.3151  | 5.1399  | 0.2748   | 1.5292   | 164.934  | 3.4873   |
| Rb1+  | 17.5816   | 1.7139   | 7.6598  | 14.7957  | 5.8981  | 0.1603   | 2.7817   | 31.2087  | 2.0782   |
| Sr    | 17.5663   | 1.5564   | 9.8184  | 14.0988  | 5.422   | 0.1664   | 2.6694   | 132.376  | 2.5064   |
| Sr2+  | 18.0874   | 1.4907   | 8.1373  | 12.6963  | 2.5654  | 24.5651  | -34.193  | -0.0138  | 41.4025  |
| Y     | 17.776    | 1.4029   | 10.2946 | 12.8006  | 5.72629 | 0.125599 | 3.26588  | 104.354  | 1.91213  |
| Y3+   | 17.9268   | 1.35417  | 9.1531  | 11.2145  | 1.76795 | 22.6599  | -33.108  | -0.01319 | 40.2602  |
| Zr    | 17.8765   | 1.27618  | 10.948  | 11.916   | 5.41732 | 0.117622 | 3.65721  | 87.6627  | 2.06929  |
| Zr4+  | 18.1668   | 1.2148   | 10.0562 | 10.1483  | 1.01118 | 21.6054  | -2.6479  | -0.10276 | 9.41454  |
| Nb    | 17.6142   | 1.18865  | 12.0144 | 11.766   | 4.04183 | 0.204785 | 3.53346  | 69.7957  | 3.75591  |
| Nb3+  | 19.8812   | 0.019175 | 18.0653 | 1.13305  | 1.01177 | 10.1621  | 1.94715  | 28.3389  | -12.912  |
| Nb5+  | 17.9163   | 1.12446  | 13.3417 | 0.028781 | 10.799  | 9.28206  | 0.337905 | 25.7228  | -6.3934  |
| Mo    | 3.7025    | 0.2772   | 17.2356 | 1.0958   | 12.8876 | 11.004   | 3.7429   | 61.6584  | 4.3875   |
| Mo3+  | 21.1664   | 0.014734 | 18.2017 | 1.03031  | 11.7423 | 9.53659  | 2.30951  | 26.6307  | -14.421  |
| Mo5+  | 21.0149   | 0.014345 | 18.0992 | 1.02238  | 11.4632 | 8.78809  | 0.740625 | 23.3452  | -14.316  |
| Mo6+  | 17.8871   | 1.03649  | 11.175  | 8.48061  | 6.57891 | 0.058881 | 0        | 0        | 0.349491 |
| Tc    | 19.1301   | 0.864132 | 11.0948 | 8.14487  | 4.64901 | 21.5707  | 2.71263  | 86.8472  | 5.40428  |
| Ru    | 19.2674   | 0.80852  | 12.9182 | 8.43467  | 4.86337 | 24.7997  | 1.56756  | 94.2928  | 5.37874  |
| Ru3+  | 18.5638   | 0.847329 | 13.2885 | 8.37164  | 9.32602 | 0.017662 | 3.00964  | 22.887   | -3.1892  |
| Ru4+  | 18.5003   | 0.844582 | 13.1787 | 8.12534  | 4.71304 | 0.36495  | 2.18535  | 20.8504  | 1.42357  |
| Rh    | 19.2957   | 0.751536 | 14.3501 | 8.21758  | 4.73425 | 25.8749  | 1.28918  | 98.6062  | 5.328    |
| Rh3+  | 18.8785</ |          |         |          |         |          |          |          |          |