If you follow my blog, then you'd probably remember how I tried to write a powder X-Ray diffraction (XRD) pattern simulator quite a while back. Well, I had to drop that due to a lot of other stuff that was going on in my life and studies (was getting my Masters then). But now I'm sort of free so I can pick that back up.

So in the next few posts I will code a Powder XRD pattern simulator step-by-step. The first step to do that is to write an Atomic Form Factor calculator. This is because atomic form factor would be used to calculate the structure factor, and hence the intensity of the XRD peaks.

Atomic form factor basically gives a measure of the intensity or the amplitude of the scattered wave and depends on the kind of scattering, and hence the nature of radiation incident. Since, I am coding an XRD simulator so we'll only talk about the X-ray form factor. For X-ray scattering, the form factor is the Fourier transform of the electron charge density around the nucleus and is assumed to be spherically symmetric so that the value of the Fourier transform only depends on the distance from the origin in reciprocal space.

The form factor for $0 \leq q \leq 25\, A^{-1}$ is given by:

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

where the values of ai, bi and c can be obtained from the International Tables for Crystallography:
http://it.iucr.org/Cb/ch6o1v0001/
or down below.

CODE:

```
/*Form Factor Calculator
By: Manas Sharma
mail: feedback@bragitoff.com
http://bragitoff.com*/
#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+","Siv","Sival","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"};
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```

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```

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, 20.2521 , 25.8499 , 17.3595 , 26.8909 , 23.3752 , 14.0049 , 27.9074 , 19.5902 ,
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, 25.9443 , 99.1722 , 23.9533 , 105.251 , 100.613 , 26.3394 , 23.4582 , 25.2017 ,
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, 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 caclculation
        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;
}
main(){
        char elem[10];
        double q, formFactor;
        printf("Enter the atomic specie:\n");
        scanf("%s",&elem);
        printf("Enter the q:\n");
        scanf("%lf",&q);
        formFactor=formFactorCalc(q,elem);
        if(formFactor!=9898989898989898){
                printf("\n\n%s\t%lf",elem,formFactor);
        }
}
```

OUTPUT:

```
manas@ubuntu:~/XRD Simulator$ ./a.out
Enter the atomic specie:
Na
Enter the q:
5


Na      5.496019
manas@ubuntu:~/XRD Simulator$
```

Atomic Form Factor Table

Element	a 1	b 1	a 2	b 2	a 3	b 3	a 4	b 4	c
H	0.489918	20.6593	0.262003	7.74039	0.196767	49.5519	0.049879	2.20159	0.001305
H1-	0.897661	53.1368	0.565616	15.187	0.415815	186.576	0.116973	3.56709	0.002389
He	0.8734	9.1037	0.6309	3.3568	0.3112	22.9276	0.178	0.9821	0.0064
Li	1.1282	3.9546	0.7508	1.0524	0.6175	85.3905	0.4653	168.261	0.0377
Li1+	0.6968	4.6237	0.7888	1.9557	0.3414	0.6316	0.1563	10.0953	0.0167
Be	1.5919	43.6427	1.1278	1.8623	0.5391	103.483	0.7029	0.542	0.0385
Be2+	6.2603	0.0027	0.8849	0.8313	0.7993	2.2758	0.1647	5.1146	-6.1092
B	2.0545	23.2185	1.3326	1.021	1.0979	60.3498	0.7068	0.1403	-0.1932
C	2.31	20.8439	1.02	10.2075	1.5886	0.5687	0.865	51.6512	0.2156
Cval	2.26069	22.6907	1.56165	0.656665	1.05075	9.75618	0.839259	55.5949	0.286977
N	12.2126	0.0057	3.1322	9.8933	2.0125	28.9975	1.1663	0.5826	-11.529
O	3.0485	13.2771	2.2868	5.7011	1.5463	0.3239	0.867	32.9089	0.2508
O1-	4.1916	12.8573	1.63969	4.17236	1.52673	47.0179	-20.307	-0.01404	21.9412
F	3.5392	10.2825	2.6412	4.2944	1.517	0.2615	1.0243	26.1476	0.2776
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

Element	a 1	b 1	a 2	b 2	a 3	b 3	a 4	b 4	c
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	11.0177	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	0.344941
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	0.764252	14.1259	7.84438	3.32515	21.2487	-6.1989	-0.01036	11.8678
Rh4+	18.8545	0.760825	13.9806	7.62436	2.53464	19.3317	-5.6526	-0.0102	11.2835
Pd	19.3319	0.698655	15.5017	7.98929	5.29537	25.2052	0.605844	76.8986	5.26593

Element	a 1	b 1	a 2	b 2	a 3	b 3	a 4	b 4	c
Pd2+	19.1701	0.696219	15.2096	7.55573	4.32234	22.5057	0	0	5.2916
Pd4+	19.2493	0.683839	14.79	7.14833	2.89289	17.9144	-7.9492	0.005127	13.0174
Ag	19.2808	0.6446	16.6885	7.4726	4.8045	24.6605	1.0463	99.8156	5.179
Ag1+	19.1812	0.646179	15.9719	7.19123	5.27475	21.7326	0.357534	66.1147	5.21572
Ag2+	19.1643	0.645643	16.2456	7.18544	4.3709	21.4072	0	0	5.21404
Cd	19.2214	0.5946	17.6444	6.9089	4.461	24.7008	1.6029	87.4825	5.0694
Cd2+	19.1514	0.597922	17.2535	6.80639	4.47128	20.2521	0	0	5.11937
In	19.1624	0.5476	18.5596	6.3776	4.2948	25.8499	2.0396	92.8029	4.9391
In3+	19.1045	0.551522	18.1108	6.3247	3.78897	17.3595	0	0	4.99635
Sn	19.1889	5.8303	19.1005	0.5031	4.4585	26.8909	2.4663	83.9571	4.7821
Sn2+	19.1094	0.5036	19.0548	5.8378	4.5648	23.3752	0.487	62.2061	4.7861
Sn4+	18.9333	5.764	19.7131	0.4655	3.4182	14.0049	0.0193	-0.7583	3.9182
Sb	19.6418	5.3034	19.0455	0.4607	5.0371	27.9074	2.6827	75.2825	4.5909
Sb3+	18.9755	0.467196	18.933	5.22126	5.10789	19.5902	0.288753	55.5113	4.69626
Sb5+	19.8685	5.44853	19.0302	0.467973	2.41253	14.1259	0	0	4.69263
Te	19.9644	4.81742	19.0138	0.420885	6.14487	28.5284	2.5239	70.8403	4.352
I	20.1472	4.347	18.9949	0.3814	7.5138	27.766	2.2735	66.8776	4.0712
I1-	20.2332	4.3579	18.997	0.3815	7.8069	29.5259	2.8868	84.9304	4.0714
Xe	20.2933	3.9282	19.0298	0.344	8.9767	26.4659	1.99	64.2658	3.7118
Cs	20.3892	3.569	19.1062	0.3107	10.662	24.3879	1.4953	213.904	3.3352
Cs1+	20.3524	3.552	19.1278	0.3086	10.2821	23.7128	0.9615	59.4565	3.2791
Ba	20.3361	3.216	19.297	0.2756	10.888	20.2073	2.6959	167.202	2.7731
Ba2+	20.1807	3.21367	19.1136	0.28331	10.9054	20.0558	0.77634	51.746	3.02902
La	20.578	2.94817	19.599	0.244475	11.3727	18.7726	3.28719	133.124	2.14678
La3+	20.2489	2.9207	19.3763	0.250698	11.6323	17.8211	0.336048	54.9453	2.4086
Ce	21.1671	2.81219	19.7695	0.226836	11.8513	17.6083	3.33049	127.113	1.86264
Ce3+	20.8036	2.77691	19.559	0.23154	11.9369	16.5408	0.612376	43.1692	2.09013
Ce4+	20.3235	2.65941	19.8186	0.21885	12.1233	15.7992	0.144583	62.2355	1.5918
Pr	22.044	2.77393	19.6697	0.222087	12.3856	16.7669	2.82428	143.644	2.0583
Pr3+	21.3727	2.6452	19.7491	0.214299	12.1329	15.323	0.97518	36.4065	1.77132
Pr4+	20.9413	2.54467	20.0539	0.202481	12.4668	14.8137	0.296689	45.4643	1.24285
Nd	22.6845	2.66248	19.6847	0.210628	12.774	15.885	2.85137	137.903	1.98486
Nd3+	21.961	2.52722	19.9339	0.199237	12.12	14.1783	1.51031	30.8717	1.47588
Pm	23.3405	2.5627	19.6095	0.202088	13.1235	15.1009	2.87516	132.721	2.02876
Pm3+	22.5527	2.4174	20.1108	0.185769	12.0671	13.1275	2.07492	27.4491	1.19499
Sm	24.0042	2.47274	19.4258	0.196451	13.4396	14.3996	2.89604	128.007	2.20963
Sm3+	23.1504	2.31641	20.2599	0.174081	11.9202	12.1571	2.71488	24.8242	0.954586
Eu	24.6274	2.3879	19.0886	0.1942	13.7603	13.7546	2.9227	123.174	2.5745
Eu2+	24.0063	2.27783	19.9504	0.17353	11.8034	11.6096	3.87243	26.5156	1.36389
Eu3+	23.7497	2.22258	20.3745	0.16394	11.8509	11.311	3.26503	22.9966	0.759344
Gd	25.0709	2.25341	19.0798	0.181951	13.8518	12.9331	3.54545	101.398	2.4196
Gd3+	24.3466	2.13553	20.4208	0.155525	11.8708	10.5782	3.7149	21.7029	0.645089
Tb	25.8976	2.24256	18.2185	0.196143	14.3167	12.6648	2.95354	115.362	3.58324
Tb3+	24.9559	2.05601	20.3271	0.149525	12.2471	10.0499	3.773	21.2773	0.691967
Dy	26.507	2.1802	17.6383	0.202172	14.5596	12.1899	2.96577	111.874	4.29728
Dy3+	25.5395	1.9804	20.2861	0.143384	11.9812	9.34972	4.50073	19.581	0.68969
Ho	26.9049	2.07051	17.294	0.19794	14.5583	11.4407	3.63837	92.6566	4.56796
Ho3+	26.1296	1.91072	20.0994	0.139358	11.9788	8.80018	4.93676	18.5908	0.852795
Er	27.6563	2.07356	16.4285	0.223545	14.9779	11.3604	2.98233	105.703	5.92046
Er3+	26.722	1.84659	19.7748	0.13729	12.1506	8.36225	5.17379	17.8974	1.17613
Tm	28.1819	2.02859	15.8851	0.238849	15.1542	10.9975	2.98706	102.961	6.75621
Tm3+	27.3083	1.78711	19.332	0.136974	12.3339	7.96778	5.38348	17.2922	1.63929
Yb	28.6641	1.9889	15.4345	0.257119	15.3087	10.6647	2.98963	100.417	7.56672
Yb2+	28.1209	1.78503	17.6817	0.15997	13.3335	8.18304	5.14657	20.39	3.70983
Yb3+	27.8917	1.73272	18.7614	0.13879	12.6072	7.64412	5.47647	16.8153	2.26001

Element	a 1	b 1	a 2	b 2	a 3	b 3	a 4	b 4	c
Lu	28.9476	1.90182	15.2208	9.98519	15.1	0.261033	3.71601	84.3298	7.97628
Lu3+	28.4628	1.68216	18.121	0.142292	12.8429	7.33727	5.59415	16.3535	2.97573
Hf	29.144	1.83262	15.1726	9.5999	14.7586	0.275116	4.30013	72.029	8.58154
Hf4+	28.8131	1.59136	18.4601	0.128903	12.7285	6.76232	5.59927	14.0366	2.39699
Ta	29.2024	1.77333	15.2293	9.37046	14.5135	0.295977	4.76492	63.3644	9.24354
Ta5+	29.1587	1.50711	18.8407	0.116741	12.8268	6.31524	5.38695	12.4244	1.78555
W	29.0818	1.72029	15.43	9.2259	14.4327	0.321703	5.11982	57.056	9.8875
W6+	29.4936	1.42755	19.3763	0.104621	13.0544	5.93667	5.06412	11.1972	1.01074
Re	28.7621	1.67191	15.7189	9.09227	14.5564	0.3505	5.44174	52.0861	10.472
Os	28.1894	1.62903	16.155	8.97948	14.9305	0.382661	5.67589	48.1647	11.0005
Os4+	30.419	1.37113	15.2637	6.84706	14.7458	0.165191	5.06795	18.003	6.49804
Ir	27.3049	1.59279	16.7296	8.86553	15.6115	0.417916	5.83377	45.0011	11.4722
Ir3+	30.4156	1.34323	15.862	7.10909	13.6145	0.204633	5.82008	20.3254	8.27903
Ir4+	30.7058	1.30923	15.5512	6.71983	14.2326	0.167252	5.53672	17.4911	6.96824
Pt	27.0059	1.51293	17.7639	8.81174	15.7131	0.424593	5.7837	38.6103	11.6883
Pt2+	29.8429	1.32927	16.7224	7.38979	13.2153	0.263297	6.35234	22.9426	9.85329
Pt4+	30.9612	1.24813	15.9829	6.60834	13.7348	0.16864	5.92034	16.9392	7.39534
Au	16.8819	0.4611	18.5913	8.6216	25.5582	1.4826	5.86	36.3956	12.0658
Au1+	28.0109	1.35321	17.8204	7.7395	14.3359	0.356752	6.58077	26.4043	11.2299
Au3+	30.6886	1.2199	16.9029	6.82872	12.7801	0.212867	6.52354	18.659	9.0968
Hg	20.6809	0.545	19.0417	8.4484	21.6575	1.5729	5.9676	38.3246	12.6089
Hg1+	25.0853	1.39507	18.4973	7.65105	16.8883	0.443378	6.48216	28.2262	12.0205
Hg2+	29.5641	1.21152	18.06	7.05639	12.8374	0.284738	6.89912	20.7482	10.6268
Tl	27.5446	0.65515	19.1584	8.70751	15.538	1.96347	5.52593	45.8149	13.1746
Tl1+	21.3985	1.4711	20.4723	0.517394	18.7478	7.43463	6.82847	28.8482	12.5258
Tl3+	30.8695	1.1008	18.3481	6.53852	11.9328	0.219074	7.00574	17.2114	9.8027
Pb	31.0617	0.6902	13.0637	2.3576	18.442	8.618	5.9696	47.2579	13.4118
Pb2+	21.7886	1.3366	19.5682	0.488383	19.1406	6.7727	7.01107	23.8132	12.4734
Pb4+	32.1244	1.00566	18.8003	6.10926	12.0175	0.147041	6.96886	14.714	8.08428
Bi	33.3689	0.704	12.951	2.9238	16.5877	8.7937	6.4692	48.0093	13.5782
Bi3+	21.8053	1.2356	19.5026	6.24149	19.1053	0.469999	7.10295	20.3185	12.4711
Bi5+	33.5364	0.91654	25.0946	0.39042	19.2497	5.71414	6.91555	12.8285	-6.7994
Po	34.6726	0.700999	15.4733	3.55078	13.1138	9.55642	7.02588	47.0045	13.677
At	35.3163	0.68587	19.0211	3.97458	9.49887	11.3824	7.42518	45.4715	13.7108
Rn	35.5631	0.6631	21.2816	4.0691	8.0037	14.0422	7.4433	44.2473	13.6905
Fr	35.9299	0.646453	23.0547	4.17619	12.1439	23.1052	2.11253	150.645	13.7247
Ra	35.763	0.616341	22.9064	3.87135	12.4739	19.9887	3.21097	142.325	13.6211
Ra2+	35.215	0.604909	21.67	3.5767	7.91342	12.601	7.65078	29.8436	13.5431
Ac	35.6597	0.589092	23.1032	3.65155	12.5977	18.599	4.08655	117.02	13.5266
Ac3+	35.1736	0.579689	22.1112	3.41437	8.19216	12.9187	7.05545	25.9443	13.4637
Th	35.5645	0.563359	23.4219	3.46204	12.7473	17.8309	4.80703	99.1722	13.4314
Th4+	35.1007	0.555054	22.4418	3.24498	9.78554	13.4661	5.29444	23.9533	13.376
Pa	35.8847	0.547751	23.2948	3.41519	14.1891	16.9235	4.17287	105.251	13.4287
U	36.0228	0.5293	23.4128	3.3253	14.9491	16.0927	4.188	100.613	13.3966
U3+	35.5747	0.52048	22.5259	3.12293	12.2165	12.7148	5.37073	26.3394	13.3092
U4+	35.3715	0.516598	22.5326	3.05053	12.0291	12.5723	4.7984	23.4582	13.2671
U6+	34.8509	0.507079	22.7584	2.8903	14.0099	13.1767	1.21457	25.2017	13.1665
Np	36.1874	0.511929	23.5964	3.25396	15.6402	15.3622	4.1855	97.4908	13.3573
Np3+	35.7074	0.502322	22.613	3.03807	12.9898	12.1449	5.43227	25.4928	13.2544
Np4+	35.5103	0.498626	22.5787	2.96627	12.7766	11.9484	4.92159	22.7502	13.2116
Np6+	35.0136	0.48981	22.7286	2.81099	14.3884	12.33	1.75669	22.6581	13.113
Pu	36.5254	0.499384	23.8083	3.26371	16.7707	14.9455	3.47947	105.98	13.3812
Pu3+	35.84	0.484938	22.7169	2.96118	13.5807	11.5331	5.66016	24.3992	13.1991
Pu4+	35.6493	0.481422	22.646	2.8902	13.3595	11.316	5.18831	21.8301	13.1555
Pu6+	35.1736	0.473204	22.7181	2.73848	14.7635	11.553	2.28678	20.9303	13.0582

Element	a 1	b 1	a 2	b 2	a 3	b 3	a 4	b 4	c
Am	36.6706	0.483629	24.0992	3.20647	17.3415	14.3136	3.49331	102.273	13.3592
Cm	36.6488	0.465154	24.4096	3.08997	17.399	13.4346	4.21665	88.4834	13.2887
Bk	36.7881	0.451018	24.7736	3.04619	17.8919	12.8946	4.23284	86.003	13.2754
Cf	36.9185	0.437533	25.1995	3.00775	18.3317	12.4044	4.24391	83.7881	13.2674

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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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