Subshell Binding Energies of Atoms and Ions from Hydrogen to Zinc.

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IPP 1/56 February 1967

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Abstract

Binding energies of electrons in the K-, L_I-, L_{III}-, M_I-, M_{III}-, M_V-, and N_I-subshells of free atoms and of ions of all ionization stages of the elements hydrogen through zinc (Z = 30) are given with full regard to experimental values.

Introduction

For the calculation of electron impact ionization cross sections [1,2] knowledge not only of the ionization potentials of atoms and ions [3] but also of binding energies of inner shell electrons is essential. Recently [4] some binding energies of the next inner subshell have been calculated as far as they could be extracted from AEL [5] or found by extrapolation.

But even for the next inner subshell there are some gaps to be filled: for ions no binding energies are known if the next inner subshell is populated by 1s-, 2p-, or 3p-electrons, though for atoms approximate values are to be found.

As the present calculation has but a rather limited accuracy, subshells L_{II}, M_{II}, and M_{IV} are not considered. For convenience the following shell notations are assumed to be equivalent: K = 1s, L_I = 2s, L_{III} = 2p, M_I = 3s, M_{III} = 3p, M_V = 3d, and N_I = 4s.

Binding energies of free atoms

Binding energies given in references 3 and 4 will not be considered here, instead a critical review of X-ray data is necessary.

For noble gases accurate data are available: the K-shell binding energy of neon was recently determined by Mehlhorn [6] (1966) to be 870.0 eV in excellent agreement with the mean value of earlier experiments surveyed in the same paper. For argon one has to combine the M_{III} binding energy of reference 3 and the term differences KM_{III} and KL_{III} given by Sandström [7] or Bearden [8,9] in order to get the K and L_{III} binding energies. The L_I binding energy of argon has been determined recently by Mehlhorn [10] (1966) to be 326.5 eV.

For the remaining elements which are by far the majority, X-ray data are available only for solids and even these sometimes were seriously in error until recently. Many tables [8,11-13] gave incorrect values for the L_I binding energies of light elements though the correct values were known well before 1950 and could be found in Landolt-Börnstein [14] and in the table given by Slater [15] (1955). Recently the correct values were reproduced by Nordberg, Hamrin, Fahlman,

Nordling and Siegbahn [16] (1966) who used the electron spectroscopic method.

Best overall consistency was achieved by Bearden and Burr [9] (1965) who used all data then available to make a least squares adjustment. Table III of their paper has been adopted therefore as a basis for the following considerations.

For the conversion of binding energies of solids into binding energies of free atoms the following statements hold approximately:

1. Energy level differences between shells are approximately the same in a solid and in a free atom.
2. Binding energies for solids which are given with respect to the Fermi level have to be augmented by the work function in order to get the energy necessary to remove the electron altogether. This energy is approximately equal to the binding energy of the respective electron in a free atom. For metals work functions are known fairly accurately.
3. For outer shells the values given in table III of reference 9 can be compared with those in references 3 and 4. Corrections thus found can be used to get approximate values for the binding energies of inner shells of a free atom by adding this correction to the values of table III in reference 9.
4. Binding energies of inner shells of free atoms give a smooth curve in a Mosley diagram as there are no chemical or solid state effects. Instead of a Mosley diagram the difference method described in reference 3 can be used.

Results achieved by applying Statement No. 2 (where applicable) or Statement No. 3 generally do not agree but differ typically by 2 eV. Statement No. 4 can be fulfilled with values lying between those found by Statement No. 2 (where applicable) and those found by Statement No. 3. Where Statement No. 2 is not applicable these values lie within $\pm$ 2 eV of Statement No. 3 with the exception of nitrogen (discrepancy: 4 eV).

The value of o.7 eV for M_I of alumin um given in table III of reference 9 is most probably misplaced, a better interpretation would be $M_{II, III}$, or a discrepancy of 5 eV would arise.

Values adopted as binding energies of free atoms are given in tables 7 through 11 together with the first and the second differences which are equivalent to the first and second derivative. The second difference is smooth everywhere except between neon and sodium and between argon and potassium, that is each time a noble gas shell is closed. The binding energies thus found differ typically by 4 eV and up to 9 eV from the values given by Slater [15].

Binding energies of ions

To demonstrate the course of the following calculations let us take table 2 with the binding energies of the 2s-electrons in the L_I-subshell as an example: the binding energies of the lithium and the beryllium sequences are identical with the ionization potentials given in reference 3, the binding energies of the boron through neon sequences are identical with the binding energies of the next inner subshell given in reference 4. The binding energies of free atoms of sodium through zinc are taken from table 8.

This leaves us with the problem to calculate binding energies for ions of the sodium through copper sequences by reasonable interpolation.

If we inspect table 2 more closely the following relations can be discovered: the difference of the binding energies of Mg I and Mg III is about two times the difference between Na I and Na II; the difference of Al I and Al IV is about three times that much, etc. This leads to the assumption that a linear interpolation between binding energies of different ionization stages of the same element could give reasonable results. The condition that the binding energies of an isoelectronic sequence should be nearly proportional to quadratic numbers can be fulfilled by this interpolation as well.

This linear interpolation works out allright up to the argon sequence. Then the above described procedure has to be repeated once more: the

difference of the binding energies of Ca I and Ca III is about two times the difference between K I and K II, the difference of Sc I and Sc IV is about three times that much, etc. In the same manner table 1 and tables 3 through 5 have been derived.

In table 6 an additional assumption had to be made concerning the M_V-subshell when a 4s-electron is present in the ground state. From AEL only approximate values can be extracted for these cases and therefore no value is given in reference 4. Here it is assumed that the M_V binding energy is approximately 1.3 eV higher than the ionization potential of the atoms Sc I through Cu I, and approximately 0.4 eV higher than the ionization potential of the ions Sc II, Ti II, Mn II, and Fe II.

Discussion

In tables 1 through 6 the results of the interpolation procedure are presented. The number of digits after the decimal point has been chosen in such a way that the last digit is uncertain by one to ten units. If a digit before the decimal point is supposed to be uncertain by more than ten units it has been underlined.

For the L_{II}-, M_{II}-, and M_{IV}-subshells no values are given because the energy difference to the L_{III}-subshell etc. is of the order of the probable error of the binding energy. For atoms the energy difference $L_{II} - L_{III}$ has been smoothed and is given in table 12.

For the conversion of wave numbers into energy the physical constants of 1963 are applied: $1\ cm^{-1} \mathrel{\hat{=}} 1.23981 \times 10^{-4}$ eV. This is true also for the X-ray data given by Bearden and Burr [9] which are used here as a basis.

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Table 1: Binding energies of 1s-electrons in the K-shell in eV.
Underlined digits are uncertain by more than 10 units.

$1\ cm^{-1} \triangleq 1.23981 \times 10^{-4}$ eV.

Z		I	II	III	IV	V	VI	VII	VIII	IX	X	XI	XII	XIII	XIV	XV	XVI	XVII	XVIII	XIX	XX	XXI	XXII	XXIII	XXIV	XXV	XXVI
1	H	13.598																									
2	He	24.587	54.416																								
3	Li	57	75.638	122.451																							
4	Be	115	125	153.888	217.713																						
5	B	192	206	220	259.363	340.217																					
6	C	288	307	325	343	392.084	489.980																				
7	N	403	426	449	471	493	552.063	667.029																			
8	O	538	564	591	618	644	670	739.327	871.387																		
9	F	694	723	753	784	815	845	875	953.900	1103.09																	
10	Ne	870.0	902	935	969	1004	1039	1073	1107	1195.82	1362.16																
11	Na	1075	1101	1137	1174	1212	1251	1290	1328	1366	1465.11	1648.66															
12	Mg	1308	1332	1360	1400	1441	1483	1526	1569	1611	1653	1761.82	1962.61														
13	Al	1564	1589	1616	1646	1690	1735	1781	1828	1875	1921	1967	2085.99	2304.1													
14	Si	1844	1871	1899	1928	1960	2008	2057	2107	2158	2209	2259	2309	2437.7	2673.1												
15	P	2148	2177	2206	2236	2267	2301	2353	2406	2460	2515	2570	2624	2678	2816.9	3069.8											
16	S	2476	2507	2538	2569	2601	2634	2670	2726	2783	2841	2900	2959	3017	3075	3223.8	3494.1										
17	Cl	2829	2860	2893	2926	2959	2993	3028	3066	3126	3187	3249	3312	3375	3437	3499	3658.3	3946									
18	A	3206.2	3237	3272	3307	3342	3377	3413	3450	3490	3554	3619	3685	3752	3819	3885	3951	4121	4426								
19	K	3610	3641	3675	3712	3749	3786	3823	3861	3900	3942	4010	4079	4149	4220	4291	4361	4431	4611	4934							
20	Ca	4041	4072	4105	4141	4180	4219	4258	4297	4337	4378	4422	4494	4567	4641	4716	4791	4865	4939	5129	5470						
21	Sc	4494	4528	4562	4597	4635	4676	4717	4758	4799	4841	4884	4930	5006	5083	5161	5240	5319	5397	5475	5675	6034					
22	Ti	4970	5007	5043	5080	5117	5157	5200	5243	5286	5329	5373	5418	5466	5546	5627	5709	5792	5875	5957	6039	6249	6626				
23	V	5470	5509	5548	5587	5626	5665	5707	5752	5797	5842	5887	5933	5980	6030	6114	6199	6285	6372	6459	6545	6631	6851	7246			
24	Cr	5994	6036	6077	6118	6159	6200	6241	6285	6332	6379	6426	6473	6521	6570	6622	6710	6799	6889	6980	7071	7161	7251	7482	7895		
25	Mn	6543	6586	6630	6673	6716	6759	6802	6845	6891	6940	6989	7038	7087	7137	7188	7242	7334	7427	7521	7616	7711	7805	7899	8141	8572	
26	Fe	7116	7161	7207	7253	7298	7343	7388	7433	7478	7526	7577	7628	7679	7730	7782	7835	7891	7987	8084	8182	8281	8380	8478	8576	8828	9278
27	Co	7714	7761	7809	7856	7904	7951	7998	8045	8092	8139	8189	8242	8295	8348	8401	8455	8510	8568	8668	8769	8871	8974	9077	9179	9281	9544
28	Ni	8337	8386	8435	8485	8534	8583	8632	8681	8730	8779	8828	8880	8935	8990	9045	9100	9156	9213	9273	9377	9482	9588	9695	9802	9908	10014
29	Cu	8985	9036	9087	9138	9189	9240	9291	9342	9393	9444	9495	9546	9600	9657	9714	9771	9828	9886	9945	10007	10116	10224	10334	10445	10556	10666
30	Zn	9662	9709	9762	9815	9868	9921	9974	10027	10080	10133	10186	10239	10292	10348	10407	10466	10525	10584	10644	10705	10769	10881	10994	11108	11223	11338

Table 2: Binding energies of 2s-electrons in the L_I-subshell.

Z		I	II	III	IV	V	VI	VII	VIII	IX	X	XI	XII	XIII	XIV	XV	XVI	XVII	XVIII	XIX	XX	XXI	XXII	XXIII	XXIV	XXV	XXVI
3	Li	5.392																									
4	Be	9.322	18.211																								
5	B	12.93	25.155	37.930																							
6	C	16.59	30.87	47.883	64.492																						
7	N	20.33	36.69	55.76	77.471	97.888																					
8	O	28.48	42.59	63.77	87.57	113.902	138.115																				
9	F	37.85	53.80	71.87	97.75	126.22	157.156	185.185																			
10	Ne	48.47	66.41	86.24	108.08	138.62	171.74	207.257	239.096																		
11	Na	67	80.09	101.96	125.67	151.18	186.36	224.12	264.199	299.851																	
12	Mg	92	103	118.76	144.45	172.01	201.14	240.98	283.38	327.985	367.456																
13	Al	121	134	147	164.47	193.86	225.20	257.9	302.4	349.51	398.621	441.94															
14	Si	154	168	183	198	217.16	250.19	285.24	321.4	370.7	422.51	476.13	523.31														
15	P	191	207	223	239	255	276.85	313.44	352.15	391.8	445.9	502.41	560.54	611.60													
16	S	232	249	266	284	302	319	343.49	383.60	425.96	469.0	527.9	589.2	651.86	706.8												
17	Cl	277	296	314	333	352	371	390	417.06	460.70	506.66	553.1	616.8	683.0	750.1	809.0											
18	A	326.5	346	366	386	406	426	447	468	497.60	544.74	594.28	644.1	712.6	783.6	855.3	918.1										
19	K	381	398	420	442	464	485	507	530	553	585.14	635.8	688.85	742.0	815.4	891.3	967.5	1034									
20	Ca	441	459	477	500	524	548	571	595	620	645	679.70	733.8	790.40	846.8	925.1	1006.0	1087	1157								
21	Sc	503	522	542	562	587	613	639	664	690	717	744	781.3	838.9	898.9	958.6	1041.8	1128	1213	1288							
22	Ti	567	588	610	632	654	681	709	737	764	792	821	850	889.9	951.0	1014.5	1077.3	1165	1256	1346	1425						
23	V	633	657	681	705	729	753	782	812	842	871	901	932	963	1005.7	1070.3	1137.1	1203	1296	1392	1486	1569					
24	Cr	702	729	755	781	807	833	859	890	922	954	985	1017	1050	1083	1128.5	1196.7	1267	1336	1434	1535	1634	1721				
25	Mn	774	804	832	860	888	916	944	972	1005	1039	1073	1106	1140	1175	1210	1258.5	1330	1404	1476	1579	1685	1788	1879			
26	Fe	850	882	912	942	972	1002	1032	1062	1092	1127	1163	1199	1234	1270	1307	1344	1396	1471	1548	1622	1731	1842	1950	2045		
27	Co	930	963	995	1027	1059	1091	1123	1155	1187	1219	1256	1294	1332	1369	1407	1446	1485	1540	1619	1699	1776	1890	2006	2119	2218	
28	Ni	1014	1047	1081	1115	1149	1183	1217	1251	1285	1319	1353	1392	1432	1472	1511	1551	1592	1633	1692	1774	1857	1938	2056	2178	2295	2398
29	Cu	1102	1134	1170	1206	1242	1278	1314	1350	1386	1422	1458	1494	1535	1577	1619	1660	1702	1745	1788	1851	1937	2023	2106	2229	2356	2478
30	Zn	1197	1232	1262	1300	1338	1376	1414	1452	1490	1528	1566	1604	1642	1685	1729	1773	1816	1860	1905	1950	2017	2107	2195	2281	2410	2542

Table 3: Binding energies of 2p-electrons in the L_{III}-subshell.

Z		I	II	III	IV	V	VI	VII	VIII	IX	X	XI	XII	XIII	XIV	XV	XVI	XVII	XVIII	XIX	XX	XXI	XXII	XXIII	XXIV	XXV	XXVI
5	B	8.298																									
6	C	11.260	24.382																								
7	N	14.532	29.600	47.438																							
8	O	13.618	35.117	54.900	77.413																						
9	F	17.422	34.970	62.661	87.10	114.242																					
10	Ne	21.564	41.081	63.45	97.10	126.19	157.933																				
11	Na	34	47.302	71.742	98.905	138.401	172.138	208.496																			
12	Mg	54	65	80.137	109.334	141.267	186.539	224.955	265.930																		
13	Al	77	90	103	119.987	153.811	190.457	241.439	284.598	330.238																	
14	Si	104	118	133	148	166.767	205.164	246.474	303.147	351.069	401.422																
15	P	134	150	166	183	199	220.469	263.373	309.333	371.689	424.387	479.50															
16	S	168	186	203	221	239	257	281.050	328.432	379.047	447.075	504.58	564.48														
17	Cl	206	225	244	263	283	303	322	348.476	400.340	455.606	529.34	591.66	656.40													
18	A	248.5	268	288	309	330	351	373	394	422.747	479.10	539.04	618.49	685.66	755.3												
19	K	296	313	335	357	380	403	426	450	473	503.896	564.73	629.36	714.56	786.6	861.1											
20	Ca	349	366	385	409	433	458	483	508	534	559	591.92	657.25	726.60	817.6	894.5	973.9										
21	Sc	403	423	443	464	490	516	543	570	597	625	652	686.82	756.7	830.8	927.5	1009.3	1094									
22	Ti	459	481	504	527	550	578	606	635	664	693	723	752	788.59	863.1	941.9	1044.4	1131	1221								
23	V	518	543	568	593	618	643	673	703	734	765	796	828	859	897.3	976.4	1060.0	1168	1260	1355							
24	Cr	579	606	634	662	689	716	743	775	807	840	873	906	940	973	1012.8	1096.7	1185	1299	1396	1496						
25	Mn	644	673	703	733	763	792	821	850	884	918	953	988	1023	1059	1094	1135.4	1224	1317	1437	1539	1644					
26	Fe	712	743	775	807	839	871	902	933	964	1000	1036	1073	1110	1147	1185	1222	1265	1358	1456	1582	1689	1799				
27	Co	784	817	850	884	918	952	986	1019	1052	1085	1123	1161	1200	1239	1278	1318	1357	1401	1500	1602	1734	1846	1962			
28	Ni	859	894	929	964	1000	1036	1072	1108	1143	1178	1213	1253	1293	1334	1375	1416	1458	1499	1545	1648	1756	1894	2010	2131		
29	Cu	937	974	1011	1048	1085	1123	1161	1199	1237	1274	1311	1348	1390	1432	1475	1518	1561	1605	1648	1695	1803	1916	2060	2182	2308	
30	Zn	1023	1057	1096	1135	1174	1213	1253	1293	1333	1373	1412	1451	1490	1534	1578	1623	1668	1713	1759	1804	1853	1966	2084	2234	2361	2492

Table 4: Binding energies of 3s-electrons in the M_I-subshell.

Z		I	II	III	IV	V	VI	VII	VIII	IX	X	XI	XII	XIII	XIV	XV	XVI	XVII	XVIII	XIX	XX
11	Na	5.139																			
12	Mg	7.646	15.035																		
13	Al	10.62	18.828	28.448																	
14	Si	13.46	22.88	33.492	45.141																
15	P	16.15	26.78	38.58	51.48	65.023															
16	S	20.20	30.69	43.8	57.60	72.68	88.051														
17	Cl	24.54	36.02	48.87	64.1	79.82	97.03	114.20													
18	A	29.24	41.74	55.49	70.4	87.6	105.19	124.51	143.45												
19	K	37	47.90	62.45	78.05	95.1	114.2	133.70	155.10	175.80											
20	Ca	46	58	70.08	86.45	103.82	123.0	144.0	165.29	188.79	211.26										
21	Sc	55	69	82	95.55	113.7	132.7	154.0	176.8	200.0	225.59	249.84									
22	Ti	64	79	94	109	124.24	144.1	164.8	188.2	212.8	237.9	265.5	291.54								
23	V	72	88	105	122	139	156.12	177.6	199.9	225.4	251.9	278.9	308.6	336.38							
24	Cr	80	98	116	135	154	172	191.16	214.3	238.3	265.8	294.0	323.0	354.7	384.4						
25	Mn	88	108	128	148	168	189	209	229.4	254.2	279.8	309.2	339.3	370.3	404.1	435.6					
26	Fe	97	118	140	162	183	205	227	249	270.8	297.2	324.3	355.8	387.8	420.8	456.6	489.9				
27	Co	106	129	152	176	199	221	245	268	292	315.4	343	372	406	439	474	512	548			
28	Ni	116	140	165	190	215	239	263	288	313	338	363.2	393	423	458	494	531	571	608		
29	Cu	126	152	178	205	231	257	283	308	334	360	387	414	445	477	514	552	591	633	672	
30	Zn	139	165	193	220	248	275	303	330	356	384	411	439	469	501	535	574	613	655	699	740

Table 5: Binding energies of 3p-electrons in the M_{III}-subshell.

Z		I	II	III	IV	V	VI	VII	VIII	IX	X	XI	XII	XIII	XIV	XV	XVI	XVII	XVIII
13	Al	5.986																	
14	Si	8.151	16.345																
15	P	10.486	19.725	30.163															
16	S	10.360	23.411	35.0	47.304														
17	Cl	12.967	23.804	39.914	53.5	67.65													
18	A	15.759	27.629	40.91	59.69	75.2	91.17												
19	K	18.72	31.71	45.81	61.11	82.66	100.0	117.83											
20	Ca	28	37	51.18	67.27	84.50	108.78	128.0	147.61										
21	Sc	33	46	58	73.930	91.9	111.0	138.0	159.0	180.5									
22	Ti	38	53	68	82	99.867	119.7	140.7	170.4	193.2	216.5								
23	V	43	60	76	93	109	128.953	150.6	173.4	205.8	230.5	255.7							
24	Cr	48	66	85	103	122	140	161.14	184.7	209.3	244.4	270.8	298.0						
25	Mn	53	73	93	113	133	154	174	196.47	221.8	248.3	286.0	314.3	343.5					
26	Fe	58	80	101	123	145	167	189	211	234.88	262.0	290.3	330.8	361.0	392.2				
27	Co	64	87	110	133	156	180	203	227	251	276.4	305	336	379	411	444			
28	Ni	72	95	119	144	168	193	218	243	268	294	321.0	352	384	430	464	499		
29	Cu	80	105	130	155	181	207	233	259	286	313	340	368.8	401	435	484	520	557	
30	Zn	90	115	142	168	194	221	249	276	304	332	361	389	419.7	454	490	542	579	619

Table 6: Binding energies of 3d-electrons in the M_V-subshell and of 4s-electrons in the N_I-subshell.

		4s = N_I		3d = M_I											
Z		I	II	I	II	III	IV	V	VI	VII	VIII	IX	X	XI	XII
19	K	4.341		-											
20	Ca	6.113	11.871	-	-										
21	Sc	6.540	12.800	8	13.3	24.758									
22	Ti	6.820	13.577	8	14.0	28.14	43.247								
23	V	6.740	-	8	14.65	29.76	48.0	65.21							
24	Cr	6.765	-	8	16.497	31.38	50.0	71.4	90.58						
25	Mn	7.434	15.640	9	16.0	33.70	52.0	73.8	98.2	119.27					
26	Fe	7.870	16.182	9	16.5	30.651	54.8	76.2	101.0	128.3	151.18				
27	Co	7.864	-	9	17.056	33.50	51.3	79.5	104	132	162	186.3			
28	Ni	7.635	-	9	18.152	35.17	54.9	75.5	108	135	165	198	224.6		
29	Cu	7.726	-	9	20.291	36.83	57.1	79.9	103	139	169	202	238	266.1	
30	Zn	9.394	17.964	11.2	24	39.71	59.4	82.6	108	134	174	206	242	281	310.8

Z		BE	Δ	Δ²
3	Li	57		
			58	
4	Be	115		19
			77	
5	B	192		19
			96	
6	C	288		19
			115	
7	N	403		20
			135	
8	O	538		21
			156	
9	F	694		20
			176	
10	Ne	870.0		29
			205	
11	Na	1075		28
			233	
12	Mg	1308		23
			256	
13	Al	1564		24
			280	
14	Si	1844		24
			304	
15	P	2148		24
			328	
16	S	2476		25
			353	
17	Cl	2829		24
			377	
18	A	3206.2		27
			404	
19	K	3610		27
			431	
20	Ca	4041		22
			453	
21	Sc	4494		23
			476	
22	Ti	4970		24
			500	
23	V	5470		24
			524	
24	Cr	5994		25
			549	
25	Mn	6543		24
			573	
26	Fe	7116		25
			598	
27	Co	7714		25
			623	
28	Ni	8337		25
			658	
29	Cu	8985		29
			677	
30	Zn	9662		

Table 7:

Binding energies of 1s-electrons in the K-shell of free atoms in eV.

Z		BE	Δ	Δ²
11	Na	67		
			25	
12	Mg	92		4
			29	
13	Al	121		4
			33	
14	Si	154		4
			37	
15	P	191		4
			41	
16	S	232		4
			45	
17	Cl	277		4.5
			49.5	
18	A	326.5		5
			54.5	
19	K	381		5.5
			60	
20	Ca	441		2
			62	
21	Sc	503		2
			64	
22	Ti	567		2
			66	
23	V	633		3
			69	
24	Cr	702		3
			72	
25	Mn	774		4
			76	
26	Fe	850		4
			80	
27	Co	930		4
			84	
28	Ni	1014		4
			88	
29	Cu	1102		7
			95	
30	Zn	1197		

Table 8:

Binding energies of 2s-electrons in the L_I-subshell of free atoms in eV.

Δ is the difference of two consecutive binding energies,

Δ^2 is the difference of two consecutive differences Δ .

Z		BE	Δ	Δ^2
11	Na	34		
			20	
12	Mg	54		3
			23	
13	Al	77		4
			27	
14	Si	104		3
			30	
15	P	134		4
			34	
16	S	168		4
			38	
17	Cl	206		4.5
			42.5	
18	A	248.5		5
			47.5	
19	K	296		5.5
			53	
20	Ca	349		1
			54	
21	Sc	403		2
			56	
22	Ti	459		3
			59	
23	V	518		2
			61	
24	Cr	579		4
			65	
25	Mn	644		3
			68	
26	Fe	712		4
			72	
27	Co	784		3
			75	
28	Ni	859		3
			78	
29	Cu	937		11
			89	
30	Zn	1023		

Table 9:

Binding energies of 2p-electrons in the L_{III}-subshell of free atoms in eV.

Z		BE	Δ
11	Na	5.1	
			2
12	Mg	7.6	
			3
13	Al	10.6	
			3
14	Si	13.5	
			3
15	P	16.2	
			4
16	S	20.2	
			4
17	Cl	24.5	
			5
18	A	29.2	
			8
19	K	37	
			9
20	Ca	46	
			9
21	Sc	55	
			9
22	Ti	64	
			8
23	V	72	
			8
24	Cr	80	
			8
25	Mn	88	
			9
26	Fe	97	
			9
27	Co	106	
			10
28	Ni	116	
			10
29	Cu	126	
			13
30	Zn	139	

Table 10:

Binding energies of 3s-electrons in the M_I-subshell of free atoms in eV.

Z		BE	Δ
19	K	18.7	
			9
20	Ca	28	
			5
21	Sc	33	
			5
22	Ti	38	
			5
23	V	43	
			5
24	Cr	48	
			5
25	Mn	53	
			5
26	Fe	58	
			6
27	Co	64	
			8
28	Ni	72	
			8
29	Cu	80	
			10
30	Zn	90	

Table 11:

Binding energies of 3p-electrons in the M_{III}-subshell of free atoms in eV.

Z		$L_{II} - L_{III}$	Δ	Δ^2
10	Ne	0.097		
			0.06	
11	Na	0.16		0.05
			0.11	
12	Mg	0.27		0.05
			0.16	
13	Al	0.43		0.06
			0.22	
14	Si	0.65		0.05
			0.27	
15	P	0.92		0.06
			0.33	
16	S	1.25		0.05
			0.38	
17	Cl	1.63		0.06
			0.44	
18	A	2.07		0.19
			0.63	
19	K	2.7		0.27
			0.9	
20	Ca	3.6		0.2
			1.1	
21	Sc	4.7		0.2
			1.3	
22	Ti	6.0		0.2
			1.5	
23	V	7.5		0.2
			1.7	
24	Cr	9.2		0.1
			1.8	
25	Mn	11.0		0.2
			2.0	
26	Fe	13.0		0.1
			2.1	
27	Co	15.1		0.2
			2.3	
28	Ni	17.4		0.2
			2.5	
29	Cu	19.95		0.6
			3.1	
30	Zn	23.1		

Table 12:

Energy difference between the L_{II} and L_{III} subshells of free atoms in eV.