Binding Energies of the Next Inner Subshell of Atoms and Ions from B to Zn.

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(in English)

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Abstract

Binding energies of the next inner subshell are given for most ionization stages of the elements boron through zinc (Z = 30). These binding energies are calculated along isoelectronic sequences with full regard to experimental values. Similarities in the periodic table are taken into account. The calculation is analogous to that used in the report IPP 1/49.

Introduction

For the calculation of electron impact ionization cross sections[1] knowledge not only of the ionization potentials of atoms and ions[2] but also of binding energies of inner shell electrons is essential. As data on these binding energies are very scarce especially for ions it was tried to calculate these from AEL[3].

To illustrate the method to be used carbon may be taken as an example: The electron configuration of atomic carbon C I is $1s^2\ 2s^2\ 2p^2$. The (first) ionization potential is defined as the energy necessary to remove one of the two 2p-electrons which is 11.260 eV. The next inner subshell here is populated by two 2s-electrons which have a 5.332 eV higher binding energy than the 2p-electrons, namely 16.592 eV. The removal of one 2s-electron results in an excited carbon ion C II of the configuration $1s^2\ 2s\ 2p^2$, the lowest term of this configuration is $^4P_{1/2}$ and the term value can be found in AEL (1958) to be 43004 $cm^{-1} \triangleq$ 5.332 eV.

The problem for carbon-like ions then is to derive a value for the term $^4P_{1/2}$ of the next higher ionization stage and to add this value to the (first) ionization potential in order to get the binding energy of the 2s-electrons. Corresponding binding energies of other atoms and ions can be found in a similar way by applying the appropriate term values.

Calculation of Term Values

For boron-like through neon-like ions and for aluminum-like through argon-like ions the next inner subshell is populated by 2s- or 3s-electrons respectively. The binding energies of these electrons can be extracted from AEL by converting the above mentioned term values into electron volts with the conversion factor $1\ cm^{-1} \triangleq 1.23981 \times 10^{-4}$ eV. Missing values can be calculated along isoelectronic sequences by the difference method described in the report IPP 1/49[2].

In table 2 to 13 term values not specially marked are derived directly from AEL Vol.I (1948) allowing for the corrections given in Vol. II (1952) and Vol. III (1958). Values marked with a star * are from recent spectroscopic measurements. Values that are missing in AEL are underlined while values from AEL that have been found incorrect during calculations are underlined after the decimal point. These corrections are given only when the need for a correction was evident, if in doubt, the AEL values were preferred throughout.

For the Be-, B-, C-, Mg-, Al- and Si-sequence it was assumed that the "first difference" between term values is approaching a constant value near 1.8 eV. This assumption is in accordance with the few experimental data that seem to be reliable but might be questioned, more experimental data are needed to verify this assumption. A few term values are given as well in cm^{-1} in order to facilitate comparison with AEL.

The appropriate term values of the N-, O-, F-, P-, S-, and Cl-sequences are known more accurately and make extrapolations more reliable. Here the "third differences" tend to be rather small and constant.

Recent spectroscopic measurements yielded corrections to the term values of N IV[4], Si III[5], and S I[6].

Discussion

In table 1 the binding energy of the next inner subshell is given by adding the appropriate term value of table 2 to 13 to the ionization potential given in report IPP 1/49. (In table 14 a correction is given for the ionization potentials of the Si-sequence. Recently the ionization potential of N IV was determined to be[4] 77.471 eV and that of F II to be[7] 34.970 eV.)

Values not specially marked are derived directly from AEL (1958). A star * indicates that either the ionization potential or the respective term value stem from recent spectroscopic measurements. Underlining after the decimal point indicates corrections to AEL values while new values are underlined altogether.

Binding energies of next inner (sub-)shells 1s, 2p and 3p cannot be extracted from AEL with the exception of K I. Here and in similar cases autoionization from an excited level is important but the lowest autoionization level is accurately known only for K I.

References

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[4] R. Hallin, Ark. Fys. 32, 201 (1966).

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[6] Y. G. Toresson, Ark. Fys. 18, 417 (1960).

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Table 1: Binding Energies of the Next Inner Subshell.

Calculated values are underlined, recent spectroscopic values are marked with a star *.
Values not specially marked are taken from AEL (1958).

1 cm^{-1} ≙ 1.23981 x 10^{-4} eV.

Z	Element	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	12.93																									
6	C	*16.59	30.87																								
7	N	20.33	*36.69	*55.76																							
8	O	28.48	42.59	63.77	87.57																						
9	F	*37.85	*53.80	71.87	97.75	126.22																					
10	Ne	48.47	66.41	86.24	108.08	138.62	171.74																				
11	Na		80.09	101.96	125.67	151.18	186.36	224.12																			
12	Mg			118.76	144.45	172.01	201.14	240.98	283.38																		
13	Al	*10.62			164.47	193.86	225.20	257.9	302.4	349.51																	
14	Si	13.46	*22.88			217.16	250.19	285.24	321.4	370.7	422.51																
15	P	*16.15	*26.78	38.58			276.85	313.44	352.15	391.8	445.9	502.41															
16	S	20.20	30.69	43.8	57.60			343.49	383.60	425.96	469.0	527.9	589.2														
17	Cl	*24.54	36.02	48.87	64.1	79.82			417.06	460.70	506.66	553.1	616.8	683.0													
18	A	29.24	*41.74	55.49	70.4	87.6	105.19			497.60	544.74	594.28	644.1	712.6	783.6												
19	K	18.72	47.90	62.45	78.05	95.1	114.2	133.70			585.14	635.8	688.85	742.0	815.4	891.3											
20	Ca			70.08	86.45	103.82	123.0	144.0	165.29			679.70	733.8	790.40	846.8	925.1	1006.0										
21	Sc				95.55	113.7	132.7	154.0	176.8	200.0			781.3	838.9	898.9	958.6	1041.8	1128									
22	Ti					124.24	144.1	164.8	188.2	212.8	237.9			889.9	951.0	1014.5	1077.3	1165	1256								
23	V						156.12	177.6	199.9	225.4	251.9	278.9			1005.7	1070.3	1137.1	1203	1296	1392							
24	Cr							191.16	214.3	238.3	265.8	294.0	323.0			1128.5	1196.7	1267	1336	1434	1535						
25	Mn								229.4	254.2	279.8	309.2	339.3	370.3			1258.5	1330	1404	1476	1579	1685					
26	Fe									270.8	297.2	324.3	355.8	387.8	420.8			1396	1471	1548	1622	1731	1842				
27	Co										315.4	343	372	406	439	474			1540	1619	1699	1776	1890	2006			
28	Ni											363.2	393	423	458	494	531			1692	1774	1857	1938	2056	2178		
29	Cu												414	445	477	514	552	591			1851	1937	2023	2106	2229	2356	
30	Zn													469	501	535	574	613	655			2017	2107	2195	2281	2410	2542

Table 2: Be-Sequence, 2s 2p ^3P_o .

Species	E (eV)	Δ	E (cm^{-1})
Be I	2.725		21978
		1.904	
B II	4.629		37334
		1.864	
C III	6.493		52367
		1.840	
N IV	*8.333		67209
		1.822	
O V	10.155		8191_o
		1.822	
F VI	11.977		96601
		1.826	
Ne VII	13.803		11133_o
		1.825	
Na VIII	15.628		126053
		1.827	
Mg IX	17.455		140786
		1.815	
Al X	19.27		1554_{oo}
		1.82	
Si XI	21.09		1701_{oo}
		1.82	
P XII	22.91		1848_{oo}
		1.82	
S XIII	24.73		
		1.82	
Cl XIV	26.55		
		1.82	
A XV	28.37		
		1.82	
K XVI	30.19		
		1.82	
Ca XVII	32.01		
		1.82	
Sc XVIII	33,83		
		1.82	
Ti XIX	35.65		
		1.82	
V XX	37.47		
		1.82	
Cr XXI	39.29		
		1.82	
Mn XXII	41.11		
		1.82	
Fe XXIII	42.93		
		1.82	
Co XXIV	44.75		
		1.82	
Ni XXV	46.57		
		1.82	
Cu XXVI	48.39		
		1.82	
Zn XXVII	50.21		

Table 3: B-Sequence, $2s\ 2p^2\ {}^4P_{1/2}$.

Species	E (eV)	Δ	E (cm^{-1})
B I	3.571		28805
		1.761	
C II	5.332		43004
		1.759	
N III	7.091		57192
		1.775	
O IV	8.866		7151_o
		1.780	
F V	10.646		8587_o
		1.784	
Ne VI	12.43		1003_{oo}
		1.79	
Na VII	14.22		1147_{oo}
		1.80	
Mg VIII	16.02		1292_{oo}
		1.81	
Al IX	17.83		143_{8oo}
		1.82	
Si X	19.65		158_{5oo}
		1.83	
P XI	21.48		173_{3oo}
		1.83	
S XII	23.31		
		1.83	
Cl XIII	25.14		
		1.83	
A XIV	26.97		
		1.83	
K XV	28.80		
		1.83	
Ca XVI	30.63		
		1.83	
Sc XVII	32.46		
		1.83	
Ti XVIII	34.29		
		1.83	
V XIX	36.12		
		1.83	
Cr XX	37.95		
		1.83	
Mn XXI	39.78		
		1.83	
Fe XXII	41.61		
		1.83	
Co XXIII	43.44		
		1.83	
Ni XXIV	45.27		
		1.83	
Cu XXV	47.10		
		1.83	
Zn XXVI	48.93		

Table 4: C-Sequence, $2s\ 2p^3\ {}^5S_2$.

Species	E (eV)	Δ	E (cm^{-1})
C I	4.182		33735
		1.618	
N II	5.800		46785
		1.678	
O III	7.478		60312
		1.732	
F IV	9.210		7429_{o}
		1.77	
Ne V	10.98		885_{6o}
		1.80	
Na VI	12.78		1031_{oo}
		1.82	
Mg VII	14.60		1178_{oo}
		1.83	
Al VIII	16.43		132_{5oo}
		1.83	
Si IX	18.26		147_{ooo}
		1.83	
P X	20.09		162_{ooo}
		1.83	
S XI	21.92		
		1.83	
Cl XII	23.75		
		1.83	
A XIII	25.58		
		1.83	
K XIV	27.41		
		1.83	
Ca XV	29.24		
		1.83	
Sc XVI	31.07		
		1.83	
Ti XVII	32.90		
		1.83	
V XVIII	34.73		
		1.83	
Cr XIX	36.56		
		1.83	
Mn XX	38.39		
		1.83	
Fe XXI	40.22		
		1.83	
Co XXII	42.05		
		1.83	
Ni XXIII	43.88		
		1.83	
Cu XXIV	45.71		
		1.83	
Zn XXV	47.54		

Table 5: N-Sequence, $2s\ 2p^4\ {}^4P_{5/2}$.

Species	E(eV)	Δ	Δ^2
N I	10.924		
		3.934	
O II	14.858		
		3.974	
F III	18.832		
		3.963	
Ne IV	22.795		0.005
		3.968	
Na V	26.763		0.009
		3.977	
Mg VI	30.740		0.022
		3.999	
Al VII	34.739		0.027
		4.026	
Si VIII	38.765		0.031
		4.057	
P IX	42.822		0.038
		4.095	
S X	46.917		0.044
		4.139	
Cl XI	51.056		0.050
		4.189	
A XII	55.245		0.056
		4.245	
K XIII	59.490		0.062
		4.307	
Ca XIV	63.797		0.068
		4.375	
Sc XV	68.172		0.074
		4.449	
Ti XVI	72.621		0.080
		4.529	
V XVII	77.150		0.086
		4.615	
Cr XVIII	81.765		0.092
		4.707	
Mn XIX	86.472		0.098
		4.805	
Fe XX	91.277		0.104
		4.909	
Co XXI	96.186		0.110
		5.019	
Ni XXII	101.205		0.116
		5.135	
Cu XXIII	106.340		0.122
		5.257	
Zn XXIV	111.597		

Table 6: O-Sequence, $2s\ 2p^5\ {}^3P_2$.

Species	E(eV)	Δ	Δ^2
O I	15.655		
		4.777	
F II	20.432		
		4.896	
Ne III	25.328		
		4.884	
Na IV	30.212		0.017
		4.901	
Mg V	35.113		0.032
		4.933	
Al VI	40.046		0.047
		4.980	
Si VII	45.026		0.058
		5.038	
P VIII	50.064		0.070
		5.108	
S IX	55.172		0.082
		5.190	
Cl X	60.362		0.094
		5.284	
A XI	65.646		0.106
		5.390	
K XII	71.036		0.118
		5.508	
Ca XIII	76.544		0.130
		5.638	
Sc XIV	82.182		0.142
		5.780	
Ti XV	87.962		0.154
		5.934	
V XVI	93.896		0.166
		6.100	
Cr XVII	99.996		0.178
		6.278	
Mn XVIII	106.274		0.190
		6.468	
Fe XIX	112.742		0.202
		6.670	
Co XX	119.412		0.214
		6.884	
Ni XXI	126.296		0.226
		7.110	
Cu XXII	133.406		0.238
		7.348	
Zn XXIII	140.754		

Table 7: F-Sequence, $2s\ 2p^6\ {}^2S_{1/2}$.

Species	E(eV)	Δ	Δ^2
F I	21.055		
		5.855	
Ne II	26.910		
		5.877	
Na III	32.787		
		5.836	
Mg IV	38.623		0.027
		5.863	
Al V	44.486		0.049
		5.912	
Si VI	50.398		0.068
		5.980	
P VII	56.378		0.078
		6.058	
S VIII	62.436		0.095
		6.153	
Cl IX	68.589		0.111
		6.264	
A X	74.853		0.127
		6.391	
K XI	81.244		0.143
		6.534	
Ca XII	87.778		0.159
		6.693	
Sc XIII	94.471		0.175
		6.868	
Ti XIV	101.339		0.191
		7.059	
V XV	108.398		0.207
		7.266	
Cr XVI	115.664		0.223
		7.489	
Mn XVII	123.153		0.239
		7.728	
Fe XVIII	130.881		0.255
		7.983	
Co XIX	138.864		0.271
		8.254	
Ni XX	147.118		0.287
		8.541	
Cu XXI	155.659		0.303
		8.844	
Zn XXII	164.503		

Table 8: Mg-Sequence, 3s 3p ^3P_o .

Species	E(eV)	Δ	E(cm^{-1})
Mg I	2.709		21850
		1.927	
Al II	4.636		37393
		1.901	
Si III	*6.537		52725
		1.883	
P IV	8.420		67912
		1.879	
S V	10.299		83307_1
		1.869	
Cl VI	12.168		98147
		1.854	
A VII	14.022		113095
		1.844	
K VIII	15.866		127968
		1.818	
Ca IX	17.684		142635
		1.810	
Sc X	19.494		15723_o
		1.826	
Ti XI	21.32		1720_{oo}
		1.82	
V XII	23.14		1867_{oo}
		1.82	
Cr XIII	24.96		2013_{oo}
		1.82	
Mn XIV	26.78		216_{ooo}
		1.82	
Fe XV	28.60		231_{ooo}
		1.82	
Co XVI	30.42		
		1.82	
Ni XVII	32.24		
		1.82	
Cu XVIII	34.06		
		1.82	
Zn XIX	35.88		

Table 9: Al-Sequence, $3s\ 3p^2\ {}^4P_{1/2}$.

Species	E (eV)	Δ	E (cm^{-1})
Al I	3.598		29020
		1.711	
Si II	5.309		42824
		1.748	
P III	7.057		56919
		1.773	
S IV	8.83		712_{00}
		1.78	
Cl V	10.61		856_{00}
		1.79	
A VI	12.40		1000_{00}
		1.79	
K VII	14.19		1145_{00}
		1.80	
Ca VIII	15.99		1290_{00}
		1.80	
Sc IX	17.79		143_{500}
		1.81	
Ti X	19.60		
		1.80	
V XI	21.4		
		1.8	
Cr XII	23.2		
		1.8	
Mn XIII	25.0		
		1.8	
Fe XIV	26.8		
		1.8	
Co XV	28.6		
		1.8	
Ni XVI	30.4		
		1.8	
Cu XVII	32.2		
		1.8	
Zn XVIII	34.0		

Table 10: Si-Sequence, $3s\ 3p^3\ {}^5S_2$.

Species	E(eV)	Δ
Si I	4.132	
		1.534
P II	5.666	
		1.614
S III	7.28	
		1.68
Cl IV	8.96	
		1.73
A V	10.69	
		1.76
K VI	12.45	
		1.78
Ca VII	14.23	
		1.79
Sc VIII	16.02	
		1.8
Ti IX	17.8	
		1.8
V X	19.6	
		1.8
Cr XI	21.4	
		1.8
Mn XII	23.2	
		1.8
Fe XIII	25.0	
		1.8
Co XIV	26.8	
		1.8
Ni XV	28.6	
		1.8
Cu XVI	30.4	
		1.8
Zn XVII	32.2	

Table 11: P-Sequence, $3s\ 3p^4\ {}^4P_{5/2}$.

Species	E(eV)	Δ	Δ^2
P I	7.381		
		2.462	
S II	9.843		
		2.372	
Cl III	12.215		
		2.361	
A IV	14.576		0.004
		2.365	
K V	16.941		0.009
		2.374	
Ca VI	19.315		0.014
		2.388	
Sc VII	21.703		0.019
		2.407	
Ti VIII	24.110		0.024
		2.431	
V IX	26.541		0.029
		2.460	
Cr X	29.001		0.034
		2.494	
Mn XI	31.495		0.039
		2.533	
Fe XII	34.028		0.044
		2.577	
Co XIII	36.605		0.049
		2.626	
Ni XIV	39.231		0.054
		2.680	
Cu XV	41.911		0.059
		2.739	
Zn XVI	44.650		

Table 12: S-Sequence, $3s\ 3p^5\ {}^3P_2$.

Species	E(eV)	Δ	Δ^2
S I	*8.929		
		2.647	
Cl II	11.576		
		2.533	
A III	14.109		
		2.527	
K IV	16.636		0.012
		2.539	
Ca V	19.175		0.025
		2.564	
Sc VI	21.739		0.030
		2.594	
Ti VII	24.333		0.038
		2.632	
V VIII	26.965		0.046
		2.678	
Cr IX	29.643		0.054
		2.732	
Mn X	32.375		0.062
		2.794	
Fe XI	35.169		0.070
		2.864	
Co XII	38.033		0.078
		2.942	
Ni XIII	40.975		0.086
		3.028	
Cu XIV	44.003		0.094
		3.122	
Zn XV	47.125		

Table 13: Cl-Sequence, $3s\ 3p^6\ {}^2S_{1/2}$.

Species	E(eV)	Δ	Δ^2
Cl I	10.77		
		2.71	
A II	13.479		
		2.714	
K III	16.193		
		2.705	
Ca IV	18.898		0.021
		2.726	
Sc V	21.624		0.027
		2.753	
Ti VI	24.377		0.042
		2.795	
V VII	27.172		0.053
		2.848	
Cr VIII	30.020		0.064
		2.912	
Mn IX	32.932		0.075
		2.987	
Fe X	35.919		0.086
		3.073	
Co XI	38.992		0.097
		3.170	
Ni XII	42.162		0.108
		3.278	
Cu XIII	45.440		0.119
		3.397	
Zn XIV	48.837		

Table 14: Si-Sequence, $3p^2\ ^3P_o$.
Corrected ionization potentials
(see IPP 1/49, Table 15).

Species	IP	Δ(Na)	Δ^2
Si I	8.151	3.012	
P II	*19.725	4.690	1.678
S III	35.0	6.55	1.86
Cl IV	53.5	8.36	1.81
A V	75.2	10.18	1.82
K VI	100.0	12.0	1.82
Ca VII	128.0	13.8	1.8
Sc VIII	159.0	15.6	1.8
Ti IX	193.2	17.4	1.8
V X	230.5	19.2	1.8
Cr XI	270.8	21.0	1.8
Mn XII	314.3	22.8	1.8
Fe XIII	361.0	24.6	1.8
Co XIV	411	26.4	1.8
Ni XV	464	28.2	1.8
Cu XVI	520	30.0	1.8
Zn XVII	579	31.8	