Exploration

Fitting & Understand the Total Energy of Electron in K Shell for Z= 2 to 103

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Abstract

By considering a simplified empirical formula, we make an attempt to fit and understand the total energy of electron in K shell starting from Z=2 to 103. The empirical formula we propose and use is $E_K \cong -\left\{\left[Z-\ln(Z)\right]^2+\frac{\exp\sqrt{Z}}{17}\right\}13.6\text{ eV}$. We note that percentage of error decreases with increasing atomic number.

Keywords: Electron, K Shell, total energy, empirical formula, atomic number.

1. Introduction

In references [1, 2], K.M. Niranjana lucidly explained about the estimation of K shell binding energy in atoms and compounds. According to modern physics, the orbiting electrons in the atoms are in definite and discrete energy levels called shells. These shells are named by letters K, L, M, N, in the increasing order of energy. Each shell has sub shells based on the angular momentum they possess viz. L(L1,L2,L3), M (M1,M2,M3,M4,M5) and so on. A neutral atom with Z number of protons in its nucleus will have same Z number of electrons. As electrons are spin-half particles, fermions, no two electrons will be in same quantum state. Hence, these electrons start occupying from the lowest energy level till all electrons get filled. The energy level below which all levels are filled by electrons is called as Fermi level. Above this lies the 'unoccupied levels'. As the energy level increases, due to the fall in electric field strength of the nucleus proportional to the inverse square of the distance and by the wave function considerations, the energy separation between subsequent levels decreases very rapidly. At large energy the spacing is so small that it can be considered as the continuum.

Consider the inner most shell electron, the K shell electron. Let the difference between Fermi energy of the atom and the K shell energy be E_K. If we incident a photon with energy less than E_K onto it, as the energy is not sufficient to excite the K shell electron to any unoccupied level, the K shell electrons will not absorb the photon but can only undergo scattering. If the photon energy is equal to E_K, the K shell electron absorbs the photon and moves to the lowest unoccupied level which is just above the Fermi level. If the photon energy is greater than E_K, the K shell electron absorbs the photon and comes out with kinetic energy equal to $\left(h\nu - E_K\right)$, where h is the Plank's constant, ν is the frequency associated with the photon and $h\nu$ is energy of the

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photon. This sort of absorption is a knock out and one to one process in which an electron readily absorbs a photon, a quantum of energy (energy packet), and comes out with an increased amount of energy (possessed by the photon). This phenomenon is called as photoelectric absorption [1]. This energy E_K which is required to remove the K shell electron from the atom or the energy needed to move an electron from the inner shell to the lowest unoccupied level is called as K shell binding energy or the K edge. The name ‘edge’ comes because of the edge like structure in the x-ray absorption spectra due to the photoelectric absorption which starts at E_K. It increases the photon absorption suddenly and hence the sharp edge in the transmitted spectrum.

At present many complicated theoretical models are available using by which K shell binding energy can be estimated. Anyhow, estimating total energy of electron in a many body system is very complicated and very interesting. In this paper, by considering a very simple formula, we make an attempt for fitting and understanding the total energy of electron in K shell for light, medium and heavy atoms. We plot the following two graphs for better understanding. Figure-1 shows the decreasing %error with increasing proton number and figure-2 indicates the estimated and currently recommended values of electron’s total energy in K shell.

In figure-1, one can see the validity of the proposed empirical formula. In between Z=23 and 92, error is less than 2%. Crossing Z=92, even though error is slowly increasing, it is less than 1%. In case of lighter atomic nuclides, error is around 13% at Z=5 and from there it reduces to0.3% at Z=23.

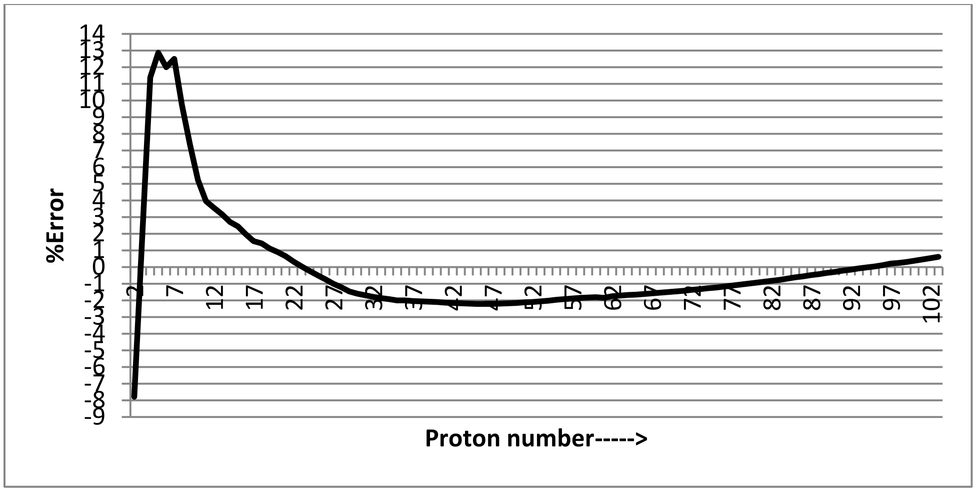

Figure 1:Decreasing %error with increasing Z

In figure-2, green line indicates the recommended values of electron’s total energy in K –shell and dotted line indicates the fitted values of electron’s total energy in K –shell. With reference to curve-fitting procedure, it is remarkable to say that, there is a fair agreement in between obtained values and recommended values and we are sure to say that, with further research and analysis, corresponding back ground physics can be understood.

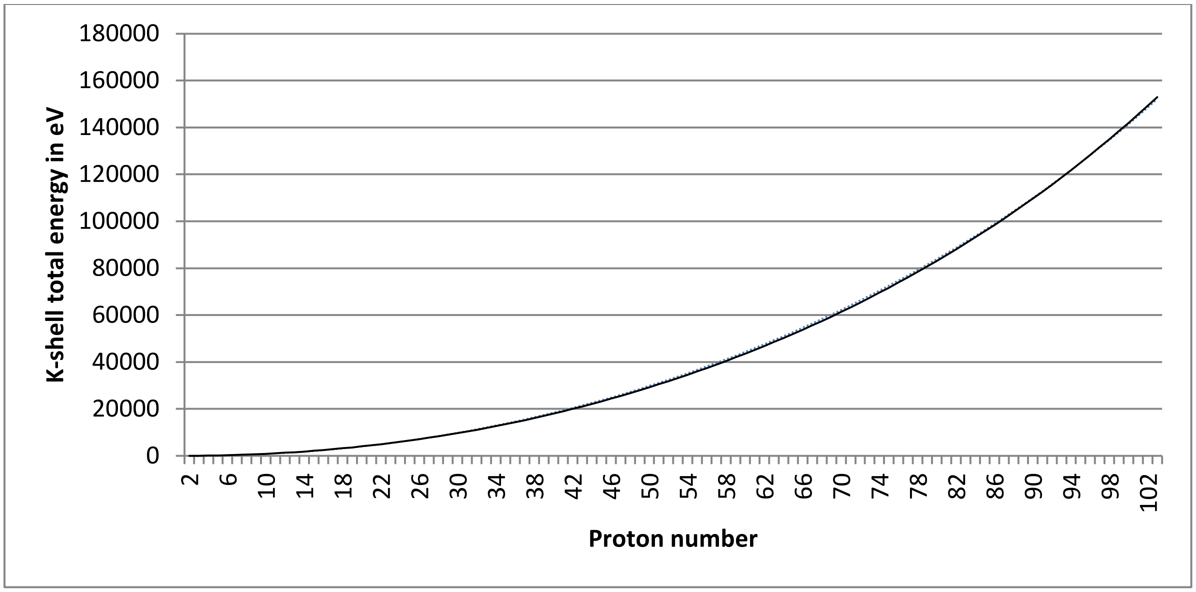

Figure 2: Electron's total energy in K shell

2. Historical review on estimating electron's binding energy

Theoretical models help us to understand any experimentally observed phenomenon by basic principles. Once the model is established, it goes further in predicting the consequences. Experiment and the theory should go hand in hand for the fruitful development of science. Ever since the experimental observation of emission lines and absorption edges, many theoretical models were built to calculate them. It was essential in understanding the atomic structure. In this journey quantum mechanics was borne. All the present theoretical approaches in this field are developed from quantum mechanical considerations. Today, we are in a position to calculate transition energies, transition probabilities, absorption edges, etc. accurately. And even we are able to determine chemical and solid state shifts, enabling better understanding of the molecular structure and dynamics. The historical review by Lindgren[3] briefly describes different theoretical models employed from past to present to calculate binding energies or absorption edges of elements and compounds.

To calculate the atomic energy levels accurately, one has to know the contributions of nuclear size, relativistic effects (corrections to Coulomb energy, magnetic and retardation energy), Coulomb and Breit correlation, radiative (QED) corrections (one- and two-electron Lamb shift, etc.) and Auger shift. It has only recently become possible to understand the relativistic many-body problem in atoms in sufficient detail to allow meaningful calculation of transition energies between hole states. Indelicato et al.[4] reported on the calculation of K, L and M inner-shell ionization energy in atoms with atomic numbers in the range $10 \leq Z \leq 100$ by evaluating many-body effects. It included correlation and effects due to the auto-ionizing nature of the hole states (Auger shift). For high Z they added recent corrected nuclear polarization, and several second-order vacuum polarization corrections. They found fairly very good agreement with the experimental edge energy measurements of gases and metal vapour. It is because, theoretical calculations are made for free atoms, not influenced by the solid state effects. One can find such fairly free atoms in gaseous state of the matter. Deslattes et al [5] combined these theoretical calculations with evaluated selected experimental data to produce a comprehensive data resource of K- and L-x-ray transition and absorption edge energies for all of the elements from neon to fermium.

The molecular many-body schemes can be categorized as follows:

1) Variational techniques, such as configuration interaction (CI) or multi-configuration self-consistent fields (MCSCF);
2) Perturbative and iterative techniques, such as many-body perturbation theory (MBPT), coupled-cluster approach (CCA) or Green's-function (GF) technique;
3) Density-functional theory (DFT).

In recent years remarkably accurate calculations have been performed of the electron binding energies of quite complicated molecules, using the density-functional theory (DFT). Takahata and Chong[6] computed core-electron binding energies of many carbon molecules using Amsterdam Density Functional Program (ADF). Segala and Chong [7] calculated K-shell core-electron binding energies for phosphorus- and sulfur-containing molecules by density functional theory to understand the chemical structure. Takahata and Marques[8] calculated accurate core-electron binding energy shifts from density functional theory for some organic compounds. There are three major classes in experimental methods to determine K shell binding energy or the K edge energy. They are,

1) X-ray Photoelectron Spectroscopy (XPS)
2) X-ray Absorption Spectroscopy (XAS)
    A) Using x-rays from a x-ray tube
    B) Using synchrotron radiation
    C) Using External Bremsstrahlung (EB) radiation from a β-ray source
3) Combining appropriate transition energies with higher shell electron binding energies

3. Semi-empirical relation for fitting electron's total energy in K shell

Independent of all of the above said complicated models and with reference to the recommended data, we developed a very simple empirical relation. It constitutes two terms.

Term-1: It depends on proton number and its natural logarithm in the following way.

$$E_{K1} \cong -\left[Z - \ln(\mathrm{Z})\right]^2 13.6 \text{ eV}. \tag{1}$$

Starting from Z= 2 to 58, approximately K- shell binding energy can be estimated.

In between Z=2 to 9, %error is around (5.5 to 17)%.

In between Z=10 and 26, %error is around (1.0 to 7.7)%.

In between Z = 27 and 49, %error is around (0.2 to 1.0)% .

Crossing Z=49, % error is gradually increasing and at Z=103, % error is 14%..

Term-2: It depends on proton number in the following way.

$$E_{K2} \cong -\left(\frac{\exp\sqrt{Z}}{17}\right)13.6 \text{ eV}. \tag{2}$$

Here, number 17 that appears in the denominator is an ad-hoc adjustable parameter and needs further review.

Total binding energy of electron in K shell can be expressed in the following way.

$$E_K \cong E_{K1} + E_{K2} \cong -\left\{\left[Z - \ln(Z)\right]^2 + \left(\frac{\exp\sqrt{Z}}{17}\right)\right\}13.6 \text{ eV}. \tag{3}$$

For data, see the following table-1.

Z	**Ln(Z)**	**Estimated** E_{K1} **eV**	**Estimated** E_{K2} **eV**	**Estimated** E_K **eV**	**Recommended** E_K **eV [9]**	**%error**
2	0.6931472	23.2	3.3	26.5	24.6	-7.79
3	1.0986123	49.2	4.5	53.7	54.7	1.85
4	1.3862944	92.9	5.9	98.8	111.5	11.37
5	1.6094379	156.3	7.5	163.8	188.0	12.86
6	1.7917595	240.8	9.3	250.1	284.2	11.99
7	1.9459101	347.4	11.3	358.7	409.9	12.50
8	2.0794415	476.7	13.5	490.3	543.1	9.73
9	2.1972246	629.4	16.1	645.4	696.7	7.36
10	2.3025851	805.8	18.9	824.7	870.2	5.23
11	2.3978953	1006.3	22.1	1028.4	1070.8	3.96
12	2.4849066	1231.3	25.6	1256.9	1303.0	3.54
13	2.5649494	1480.9	29.4	1510.3	1559.6	3.16
14	2.6390573	1755.4	33.7	1789.1	1839.0	2.71
15	2.7080502	2054.9	38.5	2093.3	2145.5	2.43
16	2.7725887	2379.5	43.7	2423.2	2472.0	1.97
17	2.8332133	2729.5	49.4	2778.9	2822.4	1.54
18	2.8903718	3104.9	55.7	3160.6	3205.9	1.41
19	2.944439	3505.8	62.5	3568.4	3608.4	1.11
20	2.9957323	3932.4	70.0	4002.4	4038.5	0.89
21	3.0445224	4384.6	78.2	4462.8	4492.0	0.65

22	3.0910425	4862.7	87.1	4949.8	4966.0	0.33
23	3.1354942	5366.5	96.8	5463.3	5465.0	0.03
24	3.1780538	5896.3	107.3	6003.6	5989.0	-0.24
25	3.2188758	6452.1	118.7	6570.8	6539.0	-0.49
26	3.2580965	7033.8	131.1	7164.9	7112.0	-0.74
27	3.2958369	7641.7	144.5	7786.1	7709.0	-1.00
28	3.3322045	8275.6	158.9	8434.5	8333.0	-1.22
29	3.3672958	8935.7	174.5	9110.2	8979.0	-1.46
30	3.4011974	9621.9	191.3	9813.3	9659.0	-1.60
31	3.4339872	10334.4	209.5	10543.9	10367.0	-1.71
32	3.4657359	11073.2	229.0	11302.2	11103.0	-1.79
33	3.4965076	11838.2	250.0	12088.2	11867.0	-1.86
34	3.5263605	12629.5	272.5	12902.1	12658.0	-1.93
35	3.5553481	13447.2	296.8	13744.0	13474.0	-2.00
36	3.5835189	14291.3	322.7	14614.0	14326.0	-2.01
37	3.6109179	15161.7	350.6	15512.3	15200.0	-2.05
38	3.6375862	16058.5	380.4	16439.0	16105.0	-2.07
39	3.6635616	16981.8	412.3	17394.2	17038.0	-2.09
40	3.6888795	17931.6	446.5	18378.1	17998.0	-2.11
41	3.7135721	18907.8	483.0	19390.8	18986.0	-2.13
42	3.7376696	19910.5	522.0	20432.4	20000.0	-2.16
43	3.7612001	20939.7	563.6	21503.3	21044.0	-2.18
44	3.7841896	21995.4	608.0	22603.4	22117.0	-2.20
45	3.8066625	23077.7	655.3	23733.0	23220.0	-2.21
46	3.8286414	24186.6	705.7	24892.3	24350.0	-2.23
47	3.8501476	25322.0	759.4	26081.4	25514.0	-2.22
48	3.871201	26484.0	816.5	27300.5	26711.0	-2.21
49	3.8918203	27672.6	877.3	28549.9	27940.0	-2.18
50	3.912023	28887.8	941.9	29829.7	29200.0	-2.16
51	3.9318256	30129.6	1010.6	31140.2	30491.0	-2.13
52	3.9512437	31398.1	1083.5	32481.6	31814.0	-2.10
53	3.9702919	32693.2	1160.9	33854.1	33169.0	-2.07
54	3.988984	34015.0	1243.1	35258.0	34561.0	-2.02
55	4.0073332	35363.4	1330.2	36693.6	35985.0	-1.97
56	4.0253517	36738.6	1422.5	38161.1	37441.0	-1.92
57	4.0430513	38140.4	1520.3	39660.7	38925.0	-1.89
58	4.060443	39568.9	1624.0	41192.8	40443.0	-1.85
59	4.0775374	41024.1	1733.7	42757.8	41991.0	-1.83
60	4.0943446	42506.0	1849.8	44355.8	43569.0	-1.81
61	4.1108739	44014.7	1972.6	45987.3	45148.0	-1.86
62	4.1271344	45550.1	2102.5	47652.5	46834.0	-1.75

63	4.1431347	47112.2	2239.7	49351.9	48519.0	-1.72
64	4.1588831	48701.0	2384.8	51085.8	50239.0	-1.69
65	4.1743873	50316.7	2538.0	52854.6	51996.0	-1.65
66	4.1896547	51959.1	2699.7	54658.8	53789.0	-1.62
67	4.2046926	53628.2	2870.4	56498.6	55618.0	-1.58
68	4.2195077	55324.1	3050.5	58374.7	57486.0	-1.55
69	4.2341065	57046.8	3240.5	60287.3	59390.0	-1.51
70	4.2484952	58796.3	3440.8	62237.1	61332.0	-1.48
71	4.2626799	60572.6	3651.9	64224.5	63314.0	-1.44
72	4.2766661	62375.7	3874.4	66250.1	65351.0	-1.38
73	4.2904594	64205.6	4108.7	68314.3	67416.0	-1.33
74	4.3040651	66062.3	4355.4	70417.8	69525.0	-1.28
75	4.3174881	67945.8	4615.2	72561.0	71676.0	-1.23
76	4.3307333	69856.2	4888.6	74744.7	73871.0	-1.18
77	4.3438054	71793.3	5176.2	76969.5	76111.0	-1.13
78	4.3567088	73757.3	5478.7	79236.0	78395.0	-1.07
79	4.3694479	75748.2	5796.7	81544.9	80725.0	-1.02
80	4.3820266	77765.9	6131.1	83897.0	83102.0	-0.96
81	4.3944492	79810.4	6482.5	86292.8	85530.0	-0.89
82	4.4067192	81881.8	6851.6	88733.4	88005.0	-0.83
83	4.4188406	83980.0	7239.4	91219.4	90524.0	-0.77
84	4.4308168	86105.1	7646.5	93751.6	93105.0	-0.69
85	4.4426513	88257.0	8074.0	96331.0	95730.0	-0.63
86	4.4543473	90435.8	8522.6	98958.4	98404.0	-0.56
87	4.4659081	92641.5	8993.3	101634.8	101137.0	-0.49
88	4.4773368	94874.1	9487.1	104361.2	103922.0	-0.42
89	4.4886364	97133.5	10005.0	107138.5	106755.0	-0.36
90	4.4998097	99419.8	10548.0	109967.8	109651.0	-0.29
91	4.5108595	101733.1	11117.2	112850.2	112601.0	-0.22
92	4.5217886	104073.1	11713.8	115786.9	115606.0	-0.16
93	4.5325995	106440.1	12338.8	118779.0	118669.0	-0.09
94	4.5432948	108834.0	12993.7	121827.7	121791.0	-0.03
95	4.5538769	111254.8	13679.5	124934.3	124982.0	0.04
96	4.5643482	113702.5	14397.6	128100.1	128241.0	0.11
97	4.574711	116177.1	15149.4	131326.5	131587.0	0.20
98	4.5849675	118678.6	15936.2	134614.9	134939.0	0.24
99	4.5951199	121207.0	16759.7	137966.7	138396.0	0.31
100	4.6051702	123762.4	17621.2	141383.5	141926.0	0.38
101	4.6151205	126344.6	18522.3	144866.9	145526.0	0.45
102	4.6249728	128953.8	19464.8	148418.6	149208.0	0.53
103	4.634729	131589.9	20450.2	152040.1	152970.0	0.61

4. Conclusions

With further research including data fitting techniques, we expect that:

1) Proposed term-1 can be given some consideration in understanding the recommended data.
2) In between Z=20 and 60, recommended K shell binding seems to lie in between the magnitudes of estimated E_{K1} and estimated $E_{K.}$. Thus, proposed term-1 seems to be sufficient for understanding the K shell binding energy for Z=20 to 60.
3) $\ln(Z)$ of term-1 can be replaced with $Z^{\frac{1}{3}}$.
4) It may be possible to review and modify the proposed term-2 and accuracy can be improved.
5) A simplified theoretical model can be developed.

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