ABSOLUTE CHEMICAL HARDNESS EASILY EXPLAINS THE "ANOMALOUS" ELECTRON CONFIGURATIONS OF CR AND CU

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ABSTRACT

In this article, it is shown that absolute chemical hardness can be employed to easily show/explain/prove that d^5 and d^{10} electron configurations are indeed more stable than all (from d^1 to d^{10}) configurations. Hence, absolute hardness can be employed to explain the apparently "anomalous" and "baffling" Cr and Cu electron configurations that are sometimes "tricky" for many high school and undergraduate basic chemistry students. *[African Journal of Chemical Education—AJCE 11(1), January 2021]*

INTRODUCTION

Electron configuration is one of the most “tricky” and “baffling” themes for high school and undergraduate basic chemistry students.

Based on quantum mechanical results, the well-known electron distribution sequence 1s 2s 2p 3s 3p 4s 3d… is memorized and then must be remembered that from scandium (Z = 21) on, the sequence is, indeed, 1s 2s 2p 3s 3p 3d 4s…

Such fact can be illustrated as in Figure 1, and the explanation is that as Z increases, the “weight” of Z values on the electron wavefunctions turns closer and closer (in energy) the 4s and 3d levels and, from scandium on, 4s “surpasses” 3d.

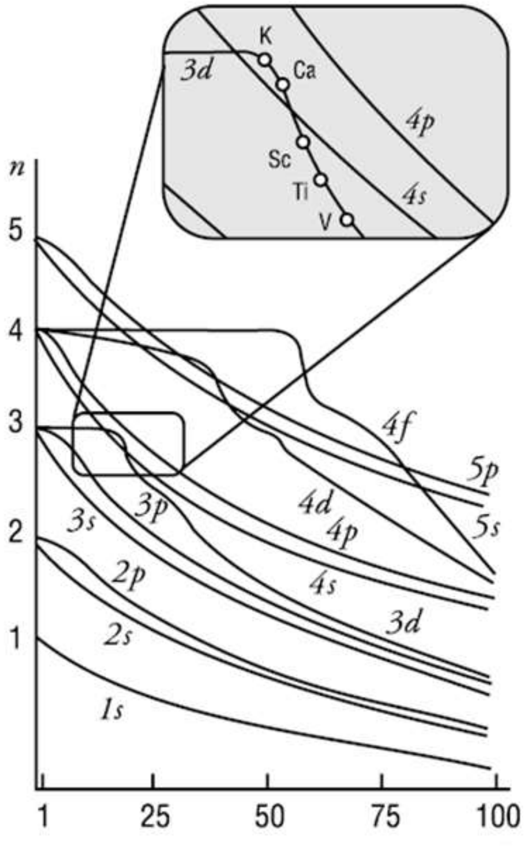

Fig. 1. Electron levels (and sublevels) as a function of atomic number (Z).

However, based on such reasoning/sequence, one must expect that Cr (Z= 24) could have the electron configuration [Ar] $3d^4 4s^2$ but it is, in fact, [Ar] $3d^5 4s^1$. Using the same reasoning, one could expect [Ar] $3d^9$ $4s^2$ for Cu (Z= 29), but it is, in fact, [Ar] $3d^{10}$ $4s^1$. Such "inversion inside the inversion" generally confuses the student.

The "official" explanation is that the half-filled subshell $3d^5$ (Cr) of full d subshell $3d^{10}$ (Cu) is most stable than the $3d^9 4s^2$ or $3d^4 4s^2$ electron configuration since in $3d^5$ and $3d^{10}$ electron configurations there are more "spherical", "symmetrical" distributions of negative charges around the nucleus and that in such cases the total energy of the system (nucleus and electrons) is downed, making it most stable.

The student ends up accepting (not without some reluctance and disbelief) this explanation. So, how to prove such reasoning? In this article, it will be shown that absolute chemical hardness can be employed to, easily, to show that $3d^5$ and $3d^{10}$ electron configuration are indeed the most stable ones.

METHODOLOGY

Absolute hardness can be calculated as $\eta = (I-A)/2$ [1] where I is the ionization energy and A is the electron affinity (both in eV). The necessary data can easily be obtained in handbooks or in reliable websites, such as RSC periodic table [2].

In Table 1 are shown the electron configurations and the absolute hardness values to some M^{2+} cations, from Sc^{2+} to Zn^{2+} [3]. Figure 2 illustrates the obtained correlation.

Table 1: Electron configurations and the absolute hardness values

Cation	Electron configuration	η/eV
Sc^{2+}	[Ar] $3d^1$	5.98
Ti^{2+}	[Ar] $3d^2$	6.96
V^{2+}	[Ar] $3d^2$	7.33
Cr^{2+}	[Ar] $3d^4$	7.23
Mn^{2+}	[Ar] $3d^5$	9.02
Fe^{2+}	[Ar] $3d^6$	7.24
Co^{2+}	[Ar] $3d^7$	8.22
Ni^{2+}	[Ar] $3d^8$	8.50
Cu^{2+}	[Ar] $3d^9$	8.27
Zn^{2+}	[Ar] $3d^{10}$	10.88

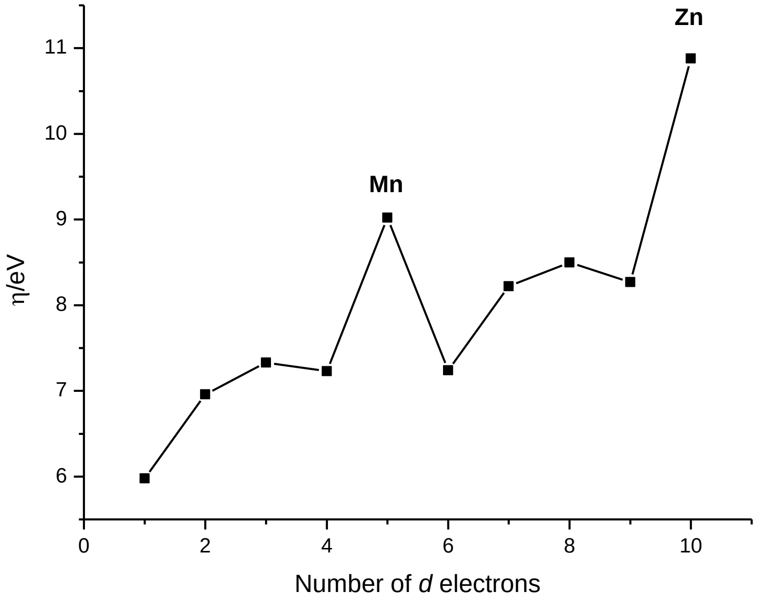

Figure 2. Absolute hardness (eV) values as a function of the number of *d* electrons to 2+ cations (from Sc^{2+} to Zn^{2+}).

RESULTS AND DISCUSSION

As can be easily seen from Table 1 data and is graphically shown in Figure 1, a half-full *d* subshell (d^5) or a full *d* subshell (d^{10}) exhibits the higher absolute hardness values from all configurations (from d^1 to d^{10}).

As is well known, higher absolute hardness values are associated with a minor frontier orbitals (HOMO and LUMO) energy difference [1] i.e., a minor polarizability.

In simple terms, in d^5 and d^{10} configurations, the electrons are more "tightly" bond to the nucleus, making the system (nucleus and electrons) most stable from an energetic point of view.

As a convincing argument, the teacher could show, to the "reluctant" student, Figure 2. As people say, "A picture is worth a thousand words".

REFERENCES

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2. https://www.rsc.org/periodic-table (consulted in March, 14, 2020).
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