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Metal cations toxicity: An inorganic interpretation

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ABSTRACT

Chemical hardness is one of the useful parameters giving information about the toxic nature of the structures. In the present work, absolute chemical hardness imparted to the science by Pearson, the hydration enthalpies, the element's electronegativity, as calculated by Batsanov (using the force constants of the bonds), the calculated electrostatic charge on the hydrated cations, the absolute radii for the metals and the effective nuclear charges, were correlated with available toxicology data for a series of metal cations (namely Hg^{2+}, Cd^{2+}, Cu^{2+} and K^{+}) in order to obtain, from a physicochemical point of view, a better understanding of the deleterious actions of metal cations on living organisms. A series of linear curves and empirical equations were obtained, providing a convincing picture of the correlation toxicity-physical inorganic chemistry.

1. Introduction

Conceptual Density Functional Theory (CDFT) [1] is among the popular theoretical tools used for the prediction of the chemical reactivity of atomic molecular chemical systems. The CDFT has introduced as a new branch by R.G. Parr as parallel to developments in Density Functional Theory of Prof Kohn [2]. In CDFT, electronegativity (χ) and chemical hardness (η) are mathematically presented as [3]:

$$\mu = -\chi = \left[\frac{\partial E}{\partial N}\right]_{\nu(r)} \tag{1}$$

$$\eta = \frac{1}{2}\left[\frac{\partial^2 E}{\partial N^2}\right]_{\nu(r)} \tag{2}$$

where, E, N and ν(r) represents the total electronic energy, the total number of electrons and constant external potential, respectively. As can be seen from the equations given, electronegativity is the negative of the chemical potential, μ. Actually, it should be noted that mathematically presentation of the chemical potential can be considered as the birth of Conceptual DFT. In the light of the finite difference approach, to calculate the electronegativity and hardness based on ground state ionization energy and electron affinities, the following formulae are obtained [4,5].

$$\chi = (I + A)/2 \tag{3}$$

$$\eta = (I - A)/2 \tag{4}$$

Within the framework of Koopmans Theorem [6], one can write

$$\chi = (-E_{HOMO} - E_{LUMO})/2 \tag{5}$$

$$\eta = (E_{LUMO} - E_{HOMO})/2 \tag{6}$$

because Koopmans Theorem states that frontier orbital energies can be used for the approximately calculation of ionization energy and electron affinities of molecular systems.

Chemical hardness is a key parameter in order to rationalize and predict chemical and physical properties of elements and compounds. For example, some researchers noted that chemical hardness is closely related to the absolute ion hydration enthalpies and some physical properties of superheavy elements [7–9]. Another study showed that chemical hardness can be considered in the prediction of hydrolysis constants for group 1 cations [10].

As is well known, metals and their compounds have long been

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recognized as important toxic agents, causing acute and chronic poisoning cases in occupational settings and in environmental high-exposure situations [11]. Many parameters can affect the toxicity of any compounds. For that reason, it is not easy to correlate with any parameter the toxic effect exhibiting when the organism is exposed to a chemical species. That is, due to the multitude of mechanisms involved and the possible target structures, metal toxicity constitutes, of course, an extremely complex field of research. Furthermore, it is necessary to take into account the biological nature of the studied subjects (mammals, plants, nematodes, bacteria, etc.) [12].

Metals play an important role in some neurobiological functions as well as being essential for healthy brain development. Metals are essential to maintain body functions through a number of biological processes. Especially, brain needs to many important transition metals like iron (Fe), cobalt (Co), manganese (Mn), copper (Cu) and zinc (Zn) to maintain its optimal physiological functions. In the central nervous system (CNS), these metals function as catalysts for biochemical reactions, gene expression regulators, second messengers in signal transduction pathways, and cofactors for many vital enzymes [13,14]. Imbalance in metal homeostasis due to metal deficiency or overload is associated with organ dysfunction leading to various diseases. Non-essential metals can have toxic effects even at low levels. The inorganic salts of various metals such as lead, mercury, tin, aluminum, and alkyl derivatives have toxic effects on behaviour and brain function [15,16].

In the literature, a few studies regarding the relation between chemical hardness and the biological actions of metals cations can be found. In the 1982, Williams and co-workers [17] by using mice and *Drosophila*, correlated metal cations toxicity (LD_{50} and LC_{50}) with chemical softness. In that work, softness values obtained by using the coordinate bond energies of fluorides and iodides were used. The aim of this article is to investigate the correlation with a series of quantum chemical parameters of toxic effects of metal ions. This paper will help to better understanding of the deleterious actions of metal cations on living organisms.

2. Methodology

LD_{50} is defined as the dose of a test substance that is lethal for 50% of the animals in a dose group. LC_{50} is the abbreviation used for the exposure concentration of a toxic substance lethal to half of the test animals. Using previously determined values [18] or making new calculations based on reference data [19] the chemical absolute hardness was obtained for a series of metal cations. The employed data are summarized in Table 1. Such absolute hardness values are will be employed to correlate with toxicity values.

All quantum chemical calculations/computations were performed by using Spartan [20]. Calculations were performed by semi-empirical (PM6) method. The SE-PM6 approach was chosen taking into account its minor computation time consuming and its reliability, as verified in the study regarding to PtF_6 [21]. Taking into account the coordination features of the considered cations, the hydrated species were modelled as follows: $[Hg(OH_2)_4]^{2+}$, $[Cd(OH_2)_4]^{2+}$, $[Cu(OH_2)_6]^{2+}$ and $[K(OH_2)_6]^{+}$.

3. Results and discussion

Absolute hardness (η) is the resistance towards electron cloud polarization or deformation of atomic and molecular chemical systems [22]. In Fig. 1, absolute hardness values (eV) for Ag^{+}, Tl^{+}, Be^{2+}, Mg^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, Sr^{2+}, Pd^{2+}, Cd^{2+}, Ba^{2+}, Pt^{2+}, Hg^{2+}, Pb^{2+}, Cr^{3+}, Fe^{3+}, Y^{3+}, Rh^{3+}, In^{3+}, Gd^{3+}, Au^{3+} and Sn^{4+} are plotted as the function of 14-day LD_{50} (mmolkg^{-1}) values obtained by Williams and co-workers [17] by using mice. As can be verified, a "V shaped" curve is obtained. In Fig. 2, a plot of 4-day LC_{50} obtained by Williams and co-workers [17] (using *Drosophila*) as function of the absolute hardness

Table 1
Chemical hardness, LD_{50} and LC_{50} and hydration enthalpy values for the investigated metal cations.

Cation	η/eV	$\Delta H_{hyd.}$/kJmol^{-1}	LD_{50}/mmolkg^{-1}[a]	LC_{50}/mM[b]
Ag^{+}	7.0	473	0.14	13
Tl^{+}	7.2	326	0.14	–
Be^{2+}	67.8	2494	0.23	45
Mg^{2+}	32.6	1921	0.41	430
Mn^{2+}	9.0	1841	0.73	42
Co^{2+}	4.5	1996	0.48	16
Ni^{2+}	8.5	2105	0.29	12
Cu^{2+}	8.3	2100	0.063	16
Zn^{2+}	10.9	2046	0.18	34
Sr^{2+}	16.3	–	4.7	32
Pd^{2+}	6.8	–	0.47	–
Cd^{2+}	10.3	1807	0.02	3.6
Ba^{2+}	12.9	1305	0.21	30
Pt^{2+}	8.0	–	0.16	–
Hg^{2+}	7.7	–	0.024	5.7
Pb^{2+}	8.5	–	0.46	_
Cr^{3+}	9.1	4560	0.8	23
Fe^{3+}	12.1	4430	1.2	_
Y^{3+}	20.0	–	0.52	25
Rh^{3+}	11.2	–	1.4	5.6
In^{3+}	13.0	–	0.04	35
Gd^{3+}	11.8	–	1.8	30
Au^{3+}	8.4	–	0.2	_
Sn^{4+}	15.6	7591	0.38	_

[a] By using mice as subjects (14-days experiment).
[b] By using *Drosophila* as subjects (4-days experiment).

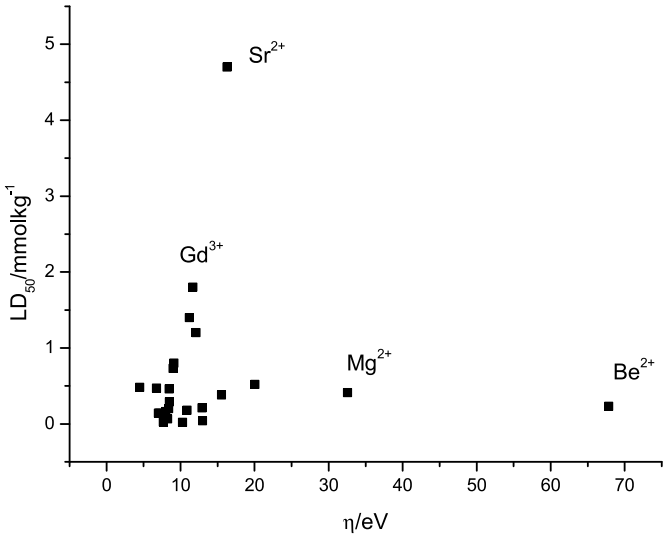

Fig. 1. LD_{50} (mmolkg^{-1}) as a function of absolute chemical hardness for Ag^{+}, Tl^{+}, Be^{2+}, Mg^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, Sr^{2+}, Pd^{2+}, Cd^{2+}, Ba^{2+}, Pt^{2+}, Hg^{2+}, Pb^{2+}, Cr^{3+}, Fe^{3+}, Y^{3+}, Rh^{3+}, In^{3+}, Gd^{3+}, Au^{3+} and Sn^{4+}.

is presented. The same "V shaped" curve is obtained. Despite the relatively complex nature of the obtained curve, this curve allows to verify that there is, indeed, a correlation between chemical hardness and LD_{50}. In order to "refine" such conclusion, another experimental data from literature should be employed, as well as a deeper physicochemical exploration should be performed. In Fig. 3, the LD_{50} values [25] are plotted as function of absolute hardness for cations with the same charge and from the same row of the periodic table: Co^{2+}, Ni^{2+} and Zn^{2+}. The curve obtained curve is a "perfect" (r = 0.9999) straight line, providing the equation

$$LD_{50} = -0.045\eta + 0.691 \quad (7)$$

When Cu^{2+} is included, the curve shown in Fig. 4 is obtained. The very higher toxicity of Cu^{2+}, in comparison with Co^{2+}, Ni^{2+} and Zn^{2+} is

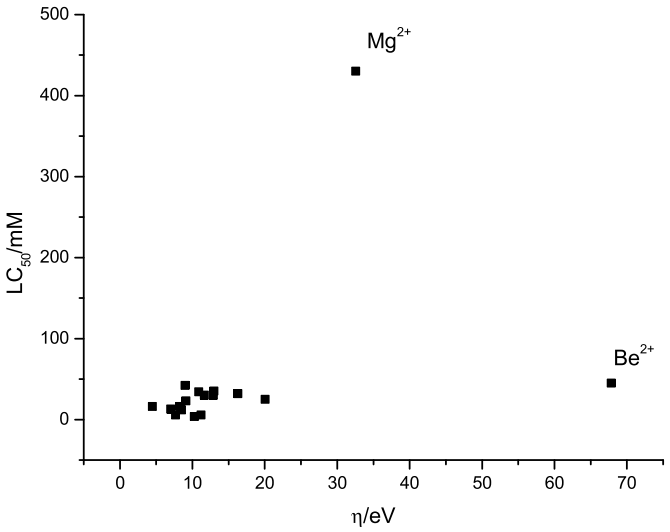

Fig. 2. LC_{50} (mM) as a function of absolute chemical hardness for Ag^{+}, Be^{2+}, Mg^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, Sr^{2+}, Cd^{2+}, Ba^{2+}, Hg^{2+}, Cr^{3+}, Y^{3+}, Rh^{3+}, In^{3+} and Gd^{3+}.

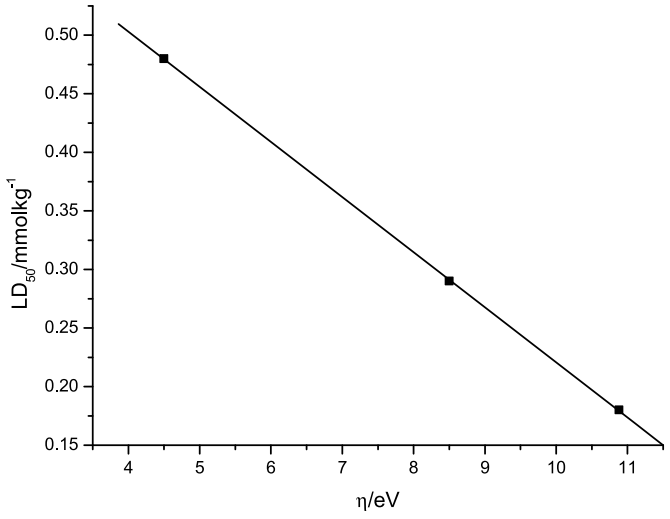

Fig. 3. LD_{50} (mmolkg^{-1}) as a function of absolute chemical hardness for Co^{2+}, Ni^{2+} and Zn^{2+}.

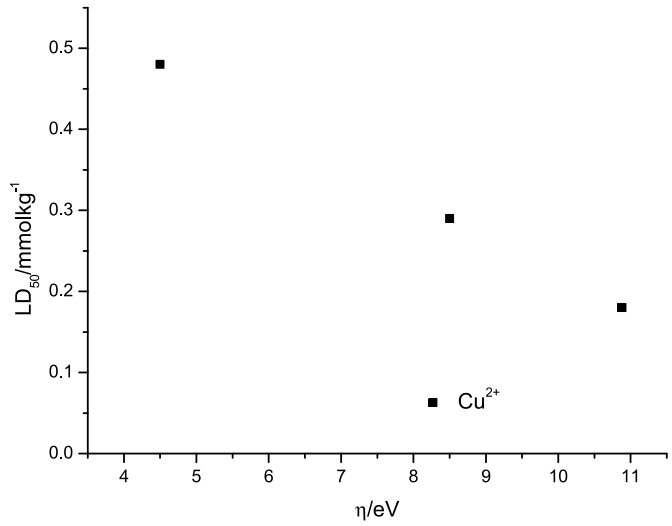

Fig. 4. LD_{50} (mmolkg^{-1}) as a function of absolute chemical hardness for Co^{2+}, Ni^{2+}, Cu^{2+} and Zn^{2+}.

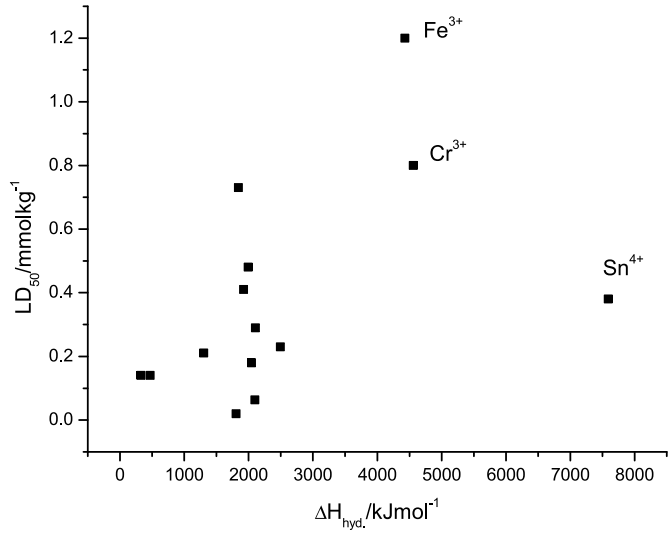

Fig. 5. LD_{50} (mmolkg^{-1}) as a function of hydration enthalpies (kJmol^{-1}) Ag^{+}, Tl^{+}, Be^{2+}, Mg^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, Cd^{2+}, Ba^{2+}, Cr^{3+}, Fe^{3+}, and Sn^{4+}.

graphically noted. Why Cu^{2+} is so highly toxic? Considering only the absolute hardness values, one can expect a toxicity closer to that of Ni^{2+}. Such "anomaly" could be attributed to the unique (in comparison with cobalt, nickel and zinc) coordination chemistry features of Cu^{2+}, due to its electronic configuration [Ar] 3 d^{9}, exhibiting the Jahn–Teller distortion [23]. In addition, it is well-known that Cu^{2+} (a borderline acid according to hard and soft acid and bases principle) has a large affinity towards nitrogen. This situation makes it very able to coordinate to nitrogenated species (in DNA, for example, causing a DNA repair inhibition). When the hydration enthalpies [24] for the metal cations are plotted as a function of their LD_{50} values [25] the curve shown in Fig. 5 is obtained. As a general trend, it is clear that higher hydration enthalpies correspond to the low values of LD_{50} (that is, higher toxicity) values. Such general trend is more clearly seen if we consider cations from the same period. In Fig. 6, LD_{50} values are plotted as a function of the hydration enthalpies (kJmol^{-1}) for Mn^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+} and Zn^{2+}. As can be seen, for such cations the higher hydration enthalpy values are associated with minor LD_{50} values, namely, with higher toxicities. These ions form strong bonds with water. The poisoning can occur when they form stronger bonds with other chemicals in living organisms than with water. As can be also verified from Fig. 5, considering only the highly (+3 and + 4) charged cations, the general trend is also verified: higher hydration enthalpy values associated with higher toxicity (lower LD_{50}).

However, if we consider only Cr^{+3} and Fe^{3+}, it is verified that higher hydrations enthalpy values are associated with higher LD50 values, that is, lower toxicity. Such fact could be explained by the fact that from a thermodynamic point of view, the cation "prefers" to retain its bonding to the oxygen atoms of water molecules instead of disrupt this linkage and make another one with other chemical substances in the living organism. In the past, it was noted that there is a remarkable correlation between absolute hardness and hydration enthalpy values [26]. Hunt and co-workers [27] performed a study using the nematode *Caenorhabditis elegans*. For 500 ppm concentration, the toxicity ranking in an initial 2-week trial was $HgCl_2 > CdCl_2 > CuCl_2 > KCl$. In Fig. 7, LD_{50} (mgkg^{-1}) for Hg^{2+}, Cd^{2+}, Cu^{2+} and K^{+} (oral doses, rats as subjects: 1, 88, 584 and 2600, respectively) are plotted as a function of the element's electronegativity, as calculated by Batsanov [28] using the force constants of the bonds (in Fig. 7, the LD50 values were obtained by using the

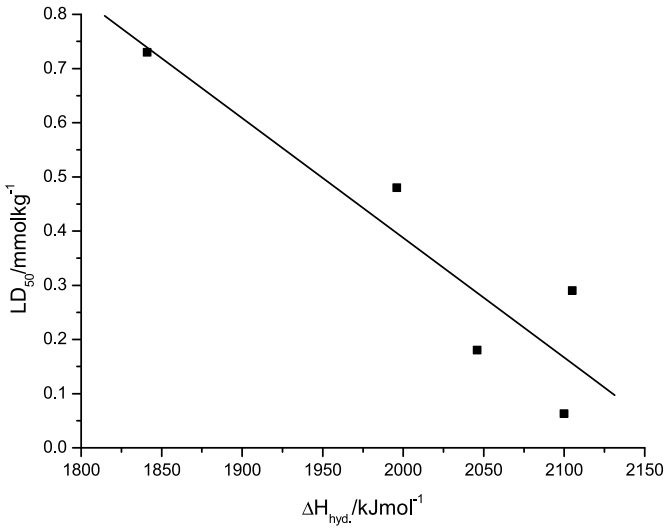

Fig. 6. LD_{50} (mmolkg^{-1}) as a function of hydration enthalpies (kJmol^{-1}) for Mn^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+} and Zn^{2+}.

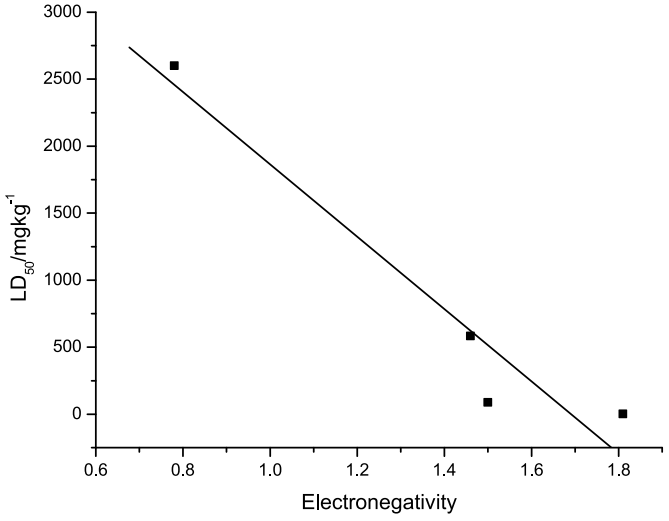

Fig. 7. LD_{50} (mgkg^{-1}) for Hg^{2+}, Cd^{2+}, Cu^{2+} and K^{+} (oral doses, rats as subjects) as a function of the electronegativity of the respective element.

respective chlorides as metal cation sources) as 1.81, 1.50, 1.46 and 0.78 for Hg, Cd, Cu and K, respectively. Such obtained curve (Fig. 7) shows, in a clear fashion, that the capacity of the element (and its respective cation) to form and disrupt chemical bonds affects, profoundly, its toxicity. If the data for Cd^{2+} is excluded, the obtained curve (r = 0.9922) provides the equation:

$$LD_{50} = -2583.48\chi + 4549.37 \quad (8)$$

So, the obtained curved and empirical equation shows clearly that the metal cations toxicity can be related with a series of well-known physicochemical parameters. In the modelled hydrated cations: $[Hg(OH_2)_4]^{2+}$, $[Cd(OH_2)_4]^{2+}$, $[Cu(OH_2)_6]^{2+}$ and $[K(OH_2)_6]^{+}$ the calculated electrostatic charge on the metal were 1.872, 1.757, 1.41 and 0.957, respectively. When the LD_{50} values (1, 88, 584 and 2600, respectively) are plotted as a function of such charges, the curve shown in Fig. 8 is obtained. In the $[Cu(OH_2)_6]^{2+}$, two axial Cu–O bonds are longer (206.2 p.m.) than the four equatorial bonds (197.7 p.m.) due the Jahn-Teller distortion. If the LD_{50} (mgkg^{-1}) for Hg^{2+}, Cd^{2+}, Cu^{2+} and K^{+} are plotted as a function of the absolute radii for the metals [29] the curve shown in Fig. 9 is obtained. a clear relationship is verified. Fig. 10

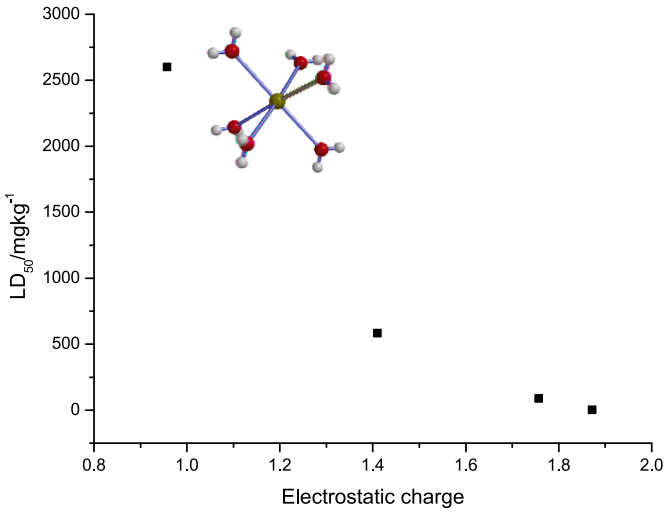

Fig. 8. LD_{50} (mgkg^{-1}) for Hg^{2+}, Cd^{2+}, Cu^{2+} and K^{+} (oral doses, rats as subjects) as a function of the calculated electrostatic charge on metal (hydrated cations). Inserted is the $[K(OH_2)_6]^{+}$ structure.

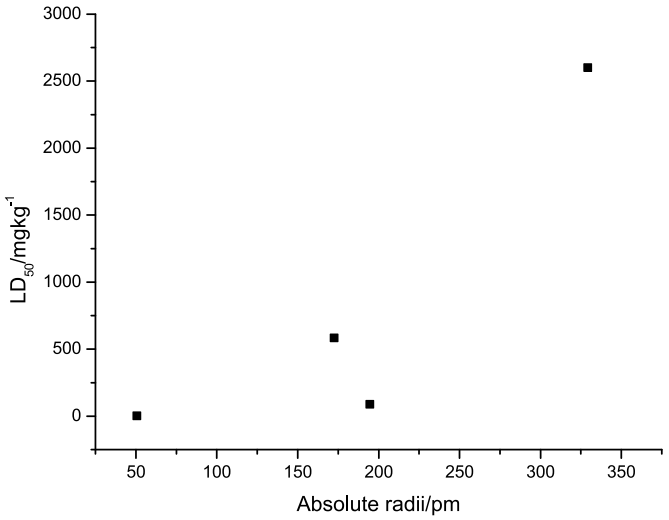

Fig. 9. LD_{50} (mgkg^{-1}) for Hg^{2+}, Cd^{2+}, Cu^{2+} and K^{+} (oral doses, rats as subjects) as a function of the absolute radii for the metals.

presents the plot of LD_{50} values as a function of the nuclear effective charge, as calculated by Clementi [30,31]. The obtained curve can be described by a first order (r = 0.9997) or second order (r = 0.9999) exponential decay. From the obtained curve it can be concluded that higher Z_{eff} values are associated with lower LD_{50} values and, of course, higher toxicities. It should be noted that in the toxicity analysis of metal cations, kinetic factors also should be considered. For example, Moyson [32] investigating the toxicity of zinc, cadmium and copper (employing *Caenorhabditis elegans* as subjects) verified that, as a general trend, the LC_{10}, LC_{20} and LC_{50} for a time of exposure of 24 h is higher than for a 48 h exposure. Furthermore, for LC_{10} and LC_{20}, the toxicity follows the sequence Cu > Cd > Zn whereas for LC_{50} the sequence is Cu > Zn > Cd. This last sequence is in agreement with the Z_{eff} values to the neutral elements: 5.84, 5.97 and 8.19 or with the Z_{eff} for the *d* electrons (that is, for the dications): 13.02, 13.89 and 15.88 for Cu, Zn and Cd, respectively.

4. Conclusion

Conceptual Density Functional Theoretical parameters such as

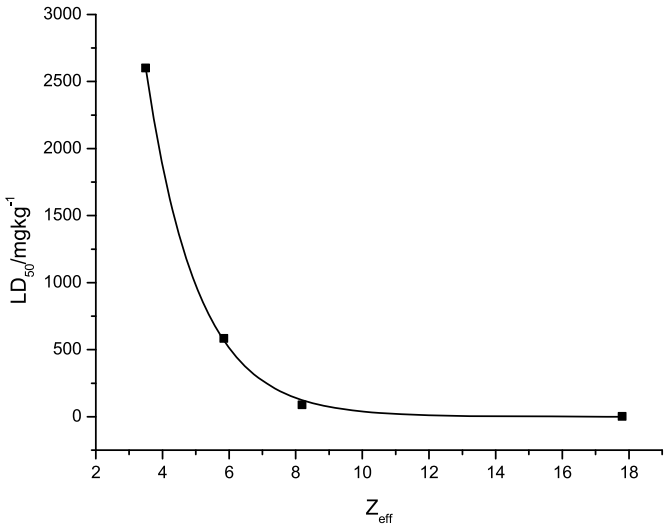

Fig. 10. LD_{50} ($mgkg^{-1}$) for Hg^{2+}, Cd^{2+}, Cu^{2+} and K^{+} (oral doses, rats as subjects) as a function of the Clementi effective nuclear charge for the metals.

electronegativity and hardness are widely used in the explanation of the chemical reactivities of atoms, ions and molecules. In the light of Hard and Soft Acid Base Principle states that "hard acids prefer to coordinate to hard bases and soft acids prefer to coordinate to soft bases", the nature of the chemical interactions can be easily explained. In the present paper, we investigated the relation with chemical hardness and electronegativity of toxicity in metal cations. It was noted that toxic nature of copper ion can be highlighted considering Jahn-Teller effect. It was noted that ionic radius and effective charge on ion are closely related to the toxicity.

5. Compliance with ethical standards

The authors report no conflicts of interest. The authors alone are responsible for the content and writing of the paper. It is not required any ethical permission because the paper doesn't include Human Participants and/or Animals.

Accompany letter to editor

All the co-authors are aware of and approve of the submission.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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