Mens Agitat, vol. 15 (2020)130-131 . ISSN 1809-4791

Super-heavy elements (Z = 110 to 120) treated as calcium clusters: ionization energies

Robson Fernandes de Farias

Universidade Federal do Rio Grande do Norte, Cx. Postal 1524, 59078-970, Natal-RN. robdefarias@yahoo.com.br

Abstract In the present work, is shown that the first ionization energies for super-heavy elements (Z= 110-120) can be calculated by a semi-empirical method, if the super-heavy atoms are treated as calcium clusters. The SE calculated values are compared with those from literature (based on relativistic quantum mechanics) with good agreement.

Keywords: Super-heavy elements, elements 110-120, calcium clusters, ionization energy, semi-empirical.

INTRODUCTION

The synthesis of the elements 111-118, increased the interest on the so called superheavy elements, been necessary to investigate/estimate/predict the properties of such elements [1-6].

Because higher Z values, trustable calculations involving the properties of super-heavy elements must, necessarily, include the relativistic contributions [7]. However, as previously shown to elements 100-109 [8], first ionization energies for super-heavy elements can be calculated by semi-empirical method, if the super-heavy atoms are treated as calcium clusters.

In the present work, such calculations are performed/extended to elements 110-120.

METHODOLOGY

All calculations were performed by using Spartan [9]. The calcium clusters were modelled as six membered rings, as previously reported [8].

Calcium was chose taking into account that ^{40}Ca has a closed nuclear shell with protons and neutrons with the so called "magic configuration", been close to the line of stability [10] as well as by the fact that calcium has been employed as "building block" for superheavy elements synthesis [11].

All calculations were performed by semi-empirical (PM6) method. The SE-PM6 approach was chose taking into account its minor computation time consuming and its reliability for calculations involving inorganic systems, as verified for PtF_6 [12] and tin borates [13]. However, to elements 110 and 118, Hartree-Fock (6-31G*) was employed, since SE method do not support noble gases.

RESULTS AND DISCUSSION

The obtained results are summarized in Table 1 and compared with calculated values from literature [2-17] (based on relativistic quantum chemical calculations or on empirical relationships).

As can be verified, the SE results are, for almost all studied elements, in good (sometimes very good) agreement with the relativistic quantum chemical values, showing that the employed approach is suitable/reliable.

As previously noted [8] for some elements, the "correct" (taking into account a reference value from literature) ionization energy value is the mean of the value calculated to the respective uncharged and cationic (+1) clusters.

To elements 110, 111, 112 and 118 the obtained results are not in good agreement with the calculated relativistic values. To elements 110 and 118, the closed shell of the noble gas in the modelled cluster could account for the under estimated values.

Table 1. First ionization energies (eV) for superheavy elements modelled as calcium clusters. The values calculated in the present work are compared with those from literature (otherwise indicated, such values from literature are based on relativistic quantum chemical calculations).

Element	Z	Modelled cluster	IE/eV (cluster)	IE/eV (ref. values)
Ds	110	Ca_5Ne^+	7.21	9.6[a]
Rg	111	Ca_5Na^+	7.65	10.6[a]
Cn	112	Ca_5Mg^+	8.67	11.97[a] 12.05[e]
Nh	113	Ca_5Al^+	6.98	7.31[a]
Fl	114	Ca_5Si^+	8.25	8.54[g] 8.63[a] 7.01[e]
Mc	115	Ca_5P	5.69	5.58[a] 5.39[e]
Lv	116	Ca_5S Ca_5S^+	4.08 8.18 6.12*	6.88[a] 7.34[d]
Ts	117	Ca_5Cl^+	7.44	7.64[a] 6.79[d]
Og	118	Ca_5Ar^+	6.70	8.91[a,g] 12.40[d]
119	119	Ca_5K Ca_5K^+	5.68 3.76 4.72*	4.04[c] 4.79[a] 4.78[b] 3.69- 3.80[c]
120	120	Ca_6 Ca_6^+	3.39 8.31 5.85*	5.84[a] 5.85[f] 4.07[d]

*Mean value of the IE calculated to the neutral and cationic (+) cluster; [a]Ref. 10; [b]Ref. 14; [c]From absolute hardness values (Ref. 3); [d]Based on estimated Clementi effective nuclear charges (Ref. 5); [f]Ref. 14; [f]CRC Handbook; [g]Ref. 17.

REFERENCES

[1] R.F. de Farias, Estimation of some physical properties for tennessine and tennessine hydride (TsH), Chem. Phys. Lett., 667 (2017) 1-3.

[2] R.F. de Farias, Estimation of the gas phase formation enthalpies for superheavy-elements (112, 113, 114, 117, 118, 119 and 120) and some of their +1 and -1 ions, Chem. Res. J., 2(3) (2017) 108-111.

[3] R.F. de Farias, The first and second ionization energies of the element 119: absolute hardness and Mulliken electronegativity for the cation 119+ based on an empirical equation involving absolute hardness, Mendeleev Commun., 28 (2018) 306-307.

[4] R.F. de Farias, Halides lattice energies and cationic hydration enthalpies for superheavy elements 119 and 120, J. Atoms and Molecules., 8(2) (2018) 1160-1165.

[5] R.F. de Farias, Estimation of Clementi effective nuclear charges and ionization energies for superheavy elements: explaining the variations for IE along period 7, J. Atoms and Molecules., 8(1) (2018) 1155-1159.

[6] R.F. de Farias, Estimating the Fermi Energies and Work Functions for the Super Heavy Elements 119 and 120 by using Cationic Absolute Hardness, Chem. Res. J., 3(2) (2018) 56-59.

[7] B.A. Hess, Relativistic effects in heavy-element chemistry and physics, Wiley, Chichester, 2003.

[8] R.F. de Farias, Super-Heavy Elements (Z = 100-109) Treated as Calcium Clusters: First Ionization Energies. ChemRxiv. Preprint., 2020. https://doi.org/10.26434/chemrxiv.12235400.v1.; Mens Agitat 15 (2020) 43-45.

[9] Wavefunction Inc., Irvine, California, USA.

[10] M. Schädel, D. Shaughnessy (eds.), The Chemistry of the Superheavy Elements (2nd ed.), Springer, Heidelberg, 2014.

[11] S. Kean, Science, A storied Russian lab is trying to push the periodic table past its limits- and uncover exotic new elements, doi:10.1126/science.aaw8425.

[12] R.F. de Farias, Computational Gas-Phase Formation Enthalpy and Electron Affinity for Platinum Hexafluoride: Is Gaseous PtF_6 Diamagnetic because of a Relativistic Effect?, Inorg. Chem., 55 (23) (2016) 12126-12127.

[13] R.F. de Farias, On the trustability of semi-empirical methods to the calculation of gas phase formation enthalpies of inorganic compounds containing heavy metals: tin borates Mor. J. Chem., 6(2) (2018) 256-258.

[14] A. Borschevsky, V. Pershina, E. Eliav, U. Kaldor, *Ab initio* predictions of atomic properties of element 120 and its lighter group-2 homologues, PHYSICAL REVIEW A 87, 022502 (2013).

[15] D. Bonchev, V. Kamenska, Predicting the properties of the 113-120 transactinide elements, J. Phys. Chem., 85 (1981) 1177-1186.

[16] CRC Handbook of chemistry and physics, 96th Ed., Taylor and Francis, Boca Raton, 2016.

[17] A. Borschevsky, V. Pershina, E. Eliav, U. Kaldor, Atomic properties of elements 114 and 118 and their adsorption on inert surfaces, EPJ Web of Conferences, 35 05002 (2012).