



## Some physicochemical properties of tennesine

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**Abstract.** By using empirical equations, several physicochemical properties to Tennesine (Ts) are estimated. Compared with available data from literature, the estimated data are reliable. The Ts-Ts bond energy and the Ts<sup>-</sup> ionic radii are also estimated.

**Keywords:** Tennesine; Electronegativity; Physical properties

### INTRODUCTION

As previously highlighted [1] to super-heavy elements, despite the theoretical/computational efforts/improvements, depending on the chosen theoretical approach, the estimated values for a series of parameters (atomic radius, polarizability, *etc.*) can vary in a wide range. Because of the absence of experimental data for the majority of so-called super-heavy elements, extrapolations and empirical equations can be a successful approach to estimate a series of properties for such elements. Hence, and ironically, the “primitive” approach used since the times of Mendeleev can be employed to decide what theoretical approach is or is not reliable.

In a previous work [2] was shown that empirical equations can be very successful, providing results in very good agreement with those obtained by sophisticated quantum relativistic calculations. By this way, I have estimated two

properties do Tennesine ( $Z = 117$ ): covalent radius and polarizability [2].

In the present work, new physicochemical properties to Tennesine are estimated.

### METHODOLOGY, RESULTS AND DISCUSSION

As is well known, there is a close relationship between the dipole moment of a given chemical bond and the difference in electronegativity between the atoms involved: the greater the difference in electronegativity, the greater the dipole moment of the bond. Thus, the electronegativity (Pauling scale) for Tennesine was estimated as follows: the electronegativity for F, C, Br, I and At were plotted as a function of the dipole moment of the H-X bond in the respective hydrides (X= F, Cl, Br, I or At) [2].

An empirical equation ( $r= 0.991$ ) was then obtained:

$$\chi = 1.084 \mu + 1.940 \quad (1)$$

where  $\mu$  is the dipole moment (Debye) of the H-X bond.

Then, using the Ts-H dipole moment: 0.24 [2], a value of 2.20 can be calculated to the electronegativity of Tennessine.

However, as previously highlighted [2] the electronegativity for Ts is expected to be lower than that for At (2.2) and H (2.2). Furthermore, the effects of relativistic contraction must be larger for Ts than for At.

Since to Tennessine  $Z = 117$ , the Lorentz Factor ( $\gamma$ ) is equal to 1.922. Hence, we can estimate a Pauling electronegativity of  $2.20/1.922 = 1.145$  to Tennessine.

In order to have a second approach, for comparison, the Pauling electronegativity to Tennessine was also calculated as follows: the X-X (X= Cl, Br, I and At) bond dissociation energies were plotted as a function of the atomic number (Z), and an empirical equation ( $r = 0.981$ ) was obtained:

$$D(X-X) = -2.762 Z + 465.981 \quad (2)$$

By using Eq. (2), a Ts-Ts bond dissociation energy of  $142.83 \text{ kJmol}^{-1}$  was calculated. By using this value, and bond dissociation energies of  $436 \text{ kJmol}^{-1}$  and  $163.03 \text{ kJmol}^{-1}$  [2] to  $\text{H}_2$  and Ts-H bonds respectively, in the well-known equation [3] (in our case, A and B are Ts and H, of course):

$$\Delta\chi = \chi_A - \chi_B = 0.102 (\Delta)^{1/2} \quad (3)$$

and an electronegativity value of 2.2 to hydrogen, the Pauling electronegativity to Tennessine was calculated as 1.053, in very good agreement with the value calculated by using Eq. (1) and taking into account the paramount relativistic contribution to Ts.

The Mulliken electronegativity can be calculated by Pauling values employing the equation [4]:

$$\chi_M = \alpha \chi_P \quad (4)$$

where  $\alpha$  is the proportionality constant as is approximately given by 2.47 eV.

Using Eq. (4), the Mulliken electronegativity to Tennessine can be calculated as 2.83.

Since Mulliken electronegativity is defined as [4]

$$\chi_M = (IP + EA)/2 \quad (5)$$

where IP is the ionization potential and EA is the electron affinity, to Tennessine,  $IP + EA = 5.66$ .

The ionization energy to Tennessine was calculated as 6.79 eV [5]. Hence, the electron affinity can be estimated as -1.13 eV. Since in Eq.(5) the "modulus" of EA and IP values are considered (positive values), a negative value to EA makes no sense from a mathematical point of view (not to

be confused with the physical fact that energy is released when an electron is added to the valence shell of an element from group 17, that is, we have an exothermic process, negative sign, therefore)

However, Pritchard [6] proposed:

$$\chi_M = 3.15 \chi_P \quad (6)$$

As a relation between Mulliken and Pauling electronegativity scales. By using Eq. (6),  $\chi_M = 3.61$ ,  $(IP + EA) = 7.22$  and  $EA = 0.43$  to Tennessine. I think this last value is more reliable.

The so-called absolute hardness is calculated as:

$$\eta = (IP - EA)/2 \quad (7)$$

hence, to Ts,  $\eta = (6.79 - 0.43)/2 = 3.18$ .

The ionic radii to  $\text{Ts}^-$  (265.85) pm was estimated as follows: the ionic radius (to coordination number 6) to  $\text{F}^-$ ,  $\text{Cl}^-$ ,  $\text{Br}^-$  and  $\text{I}^-$ , respectively 133, 181, 196 and 220 pm [7] were plotted (Fig. 1) as a function of the H-X (X= F, C, Br or I) bond distance in the respective hydrides: 91.69, 127.46, 141.45 and 160.90 pm [2].

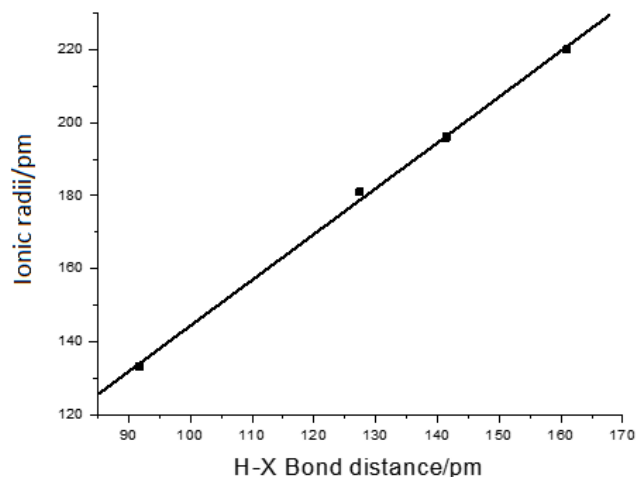


Fig.1. Ionic radii of  $\text{F}^-$ ,  $\text{Cl}^-$ ,  $\text{Br}^-$  and  $\text{I}^-$ , as a function of the H-X bond distance (X= F, C, Br or I).

An empirical equation ( $r = 0.999$ ) was obtained:

$$r = 1.256 d + 18.810 \quad (8)$$

where  $d$  is the H-X bond distance. Hence, applying to this equation the H-Ts bond distance: 196.76 pm [2], the ionic radii to  $\text{Ts}^-$  was calculated.

The Allen electronegativity to Ts was estimated as follows: the electronegativity values to Cl, Br and I (fluorine was excluded because, as is almost always the case, it exhibits,

in relation to the so-called periodic properties, an anomalous behavior in relation to the others in the group), respectively 2.869, 2.685 and 2.359 [8] were plotted as a function of Z, and an empirical equation ( $r=0.986$ ) was obtained:

$$\chi_A = -0.014 Z + 3.136 \quad (9)$$

By using this equation,  $\chi_A$  to At and Ts, can be calculated as 1.946 and 1.498, respectively. However, to At and Ts the relativistic contributions must necessarily be taken into account. Multiplying each previously  $\chi_A$  values by the Lorentz factor,  $\gamma=1.275$  (At) and 1.922 (Ts), we have:  $\chi_A=2.48$  (At) and  $\chi_A=2.88$  (Ts), in very good agreement with the first principles calculations of Karol [9]: 2.50 (At) and 2.81 (Ts).

In Table 1 we have a summary of the calculated properties to Tennessine in the present work.

Table 1. Physicochemical properties calculated (estimated) to Tennessine

Pauling electronegativity	1.15
Allen electronegativity	2.88
Mulliken electronegativity	3.61
Absolute hardness/eV	3.18
Electron affinity/eV	0.43
Ts-Ts bond energy/kJmol <sup>-1</sup>	142.83
Ts <sup>-</sup> ionic radii/pm	265.85

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