

Lattice Energies from Hydration Enthalpies: Some acid-base and Structural Considerations

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Abstract— In the present work, using reference values for the hydration enthalpies for a series of mono, di, tri and tetra cations, as well as reference values for the lattice energies of a series of mono, di, tri and tetrahalides, it is shown that reliable lattice energies for such halides can be calculated by $U_{POT} = (\Delta H_{hyd}^+ + \Delta H_{hyd}^-)$, by $U_{POT} = (\Delta H_{hyd}^+ + 2\Delta H_{hyd}^-)$, by $U_{POT} = (\Delta H_{hyd}^+ + 3\Delta H_{hyd}^-)$ or by $U_{POT} = (\Delta H_{hyd}^+ + 4\Delta H_{hyd}^-)$ for mono, di, tri and tetrahalides, respectively. Linearized improved versions of such simply equations, parametrized in order to take into account factors such as dilution and entropic contributions, were also obtained. Lattice energies for a series of halides and other salts are calculated by using the obtained empirical equations, providing results in very good agreement with literature reference values. Furthermore, a series of empirical equations were derived, relating several acid-base parameters with lattice energy. It is shown that the cation and anion volumes (obtained by X-ray data), are very closely related with the cation and anion absolute hardness, that is, are very closely related with the frontier (HOMO and LUMO) orbitals energies.

Keywords— Lattice energies, hydration enthalpies, empirical equations.

I. INTRODUCTION

Lattice energy is a prominent parameter in chemistry, since it could be related with a series of properties of a given compound, such as solubility, melting point, etc. (Dasent, 1982). Furthermore, hydration enthalpy is one of the fundamental quantities for the thermodynamics of aqueous systems.

Most recently, we have been developed an empirical equation to calculate the lattice energies for metal monohalides from average orbital electronegativities (de Farias, 2017).

In the present work, are derives empirical equation that allows the calculation of lattice energies for +1, +2, +3 and +4 salts (specially halides) based only on hydration enthalpies.

II. METHODOLOGY, RESULTS AND DISCUSSION

The up to date hydration enthalpies for group 1 monocations and group 17 monoanions (Housecroft, 2017) as well as the lattice energies (U_{POT}) to the respective halides (Glasser, 2000; Mu, 2000) are summarized in Table 1. As can be verified, the sum of cations and anion hydrations enthalpies are in very good agreement with the lattice energies for the respective metal halides. Taking into account the uncertainties that there are in both, U_{POT} and ΔH_{hyd} values, such agreement is really quite good. Hence, the following equation can be derived:

$$U_{POT} = (\Delta H_{hyd}^+ + \Delta H_{hyd}^-) \quad (1)$$

where ΔH_{hyd}^+ and ΔH_{hyd}^- are the hydration enthalpies of the respective cation and anion.

Table.1: Hydration enthalpies (kJmol^{-1}) for group 1 monocations and group 17 monoanions, and lattice energies (kJmol^{-1}) for group 1 halides.

	$-\Delta H_{hyd}^0$	$\Delta H_{hyd}^+ + \Delta H_{hyd}^-$	$U_{POT} \text{ (Ref.)}$	$\Delta\%$
Li ⁺	578.1			
Na ⁺	463.3			
K ⁺	380.3			
Rb ⁺	355.2			
Cs ⁺	330.6			
F ⁻	463.7			
Cl ⁻	319.5			
Br ⁻	288.7			
I ⁻	246.8			
LiF		1042	1030	+1.2
LiCl		898	834	+7.7
LiBr		867	788	+10.0
LiI		825	730	+13.0
NaF		927	910	+1.9
NaCl		783	769	+1.8
NaBr		752	732	+2.7
NaI		710	682	+4.1
KF		844	808	+4.6
KCl		700	701	-0.1

KBr	669	671	-0.3
KI	627	632	-0.8
RbF	819	774	+5.8
RbCl	675	680	-0.7
RbBr	644	632	+1.9
RbI	602	617	-2.4
CsF	794	759	+4.6
CsCl	650	670	-3.0
CsBr	619	647	-4.3
CsI	577	613	-5.9

When lattice energy is plotted as a function of the sum of the respective cation and anion hydration enthalpies, the curve shown in Figure 1 ($r = 0.9687$) is obtained, from which the following empirical equation is derived: .

$$U_{POT} = 0.820 (\Delta H_{hyd}^{+} + \Delta H_{hyd}^{-}) + 118.236 \quad (2)$$

Such phenomena ($U_{POT} = \Delta H_{hyd}^{+} + \Delta H_{hyd}^{-}$) can be explained if we take into account that in the solid state (where cations are surrounded by anions and anions by cations, e.g. in a 6:6 environment, as in NaCl), or in solution (where both, cations and anions are surrounded by the solvent molecules), both, cations and anions are "looking for" (thermodynamic) stability.

In these systems, stability means to interact with positive or negative species in order to equalize their electronic chemical potentials (Parr, 1978), and such stability is achieved by exothermic interactions, with the total amount of energy required by the cation (or by the anion) been the same, no matter if the interactions occurs with other anions (or cations) in the solid state or, as in aqueous solutions, with the negative (or positive) poles of the solvent molecules.

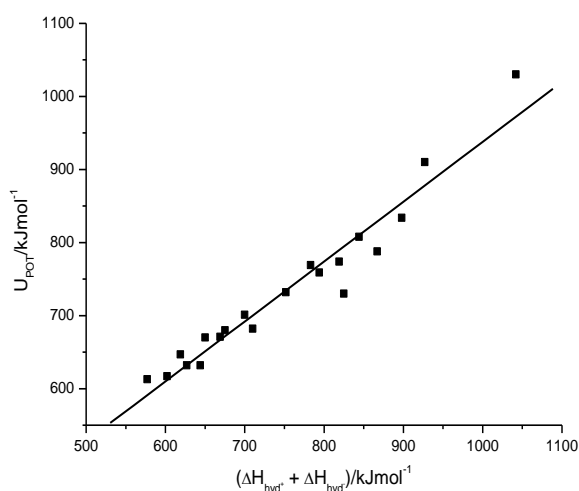


Fig. 1: Lattice energies for group 1 halides, as function of the sum of the hydration enthalpies to the respective cations and anions.

The same procedures were repeated to group 2 halides, and the respective data are summarized in Table 2. The experimental hydration enthalpies for group 2 cations are those provided by (Smith, 1977). The agreement between reference and lattice energies calculated by using the equation:

$$U_{POT} = (\Delta H_{hyd}^{+} + 2\Delta H_{hyd}^{-}) \quad (3)$$

are very good, as verified in Table 2 data, and Figure 2.

Table.2: Hydration enthalpies (kJmol^{-1}) for group 2 cations and group 17 monoanions, and lattice energies (kJmol^{-1}) for group 2 halides.

	$-\Delta H_{hyd}^0$	$\Delta H_{hyd}^{2+} + 2\Delta H_{hyd}^{-}$	$U_{POT} \text{ (Ref.)}$	$\Delta\%$
Be ²⁺	2494			
Mg ²⁺	1921			
Ca ²⁺	1577			
Sr ²⁺	1443			
Ba ²⁺	1305			
F ⁻	463.7			
Cl ⁻	319.5			
Br ⁻	288.7			
I ⁻	246.8			
BeF ₂		3421	3526	-3.0
BeCl ₂		3133	3033	+3.3
BeBr ₂		3069	2914	+5.3
BeI ₂		2988	2813	+6.2
MgF ₂		2848	2978	-4.4
MgCl ₂		2560	2540	+0.8
MgBr ₂		2498	2451	+1.9
MgI ₂		2415	2340	+3.2
CaF ₂		2504	2651	-5.5
CaCl ₂		2216	2271	-2.4
CaBr ₂		2154	2134	+0.9
CaI ₂		2071	2087	-0.8
SrF ₂		2370	2513	-5.7
SrCl ₂		2082	2170	-4.1
SrBr ₂		2020	2040	-1.0
SrI ₂		1937	1976	-2.0
BaF ₂		2232	2373	-6.2
BaCl ₂		1944	2069	-6.0
BaBr ₂		1882	1995	-5.7
BaI ₂		1799	1890	-4.8

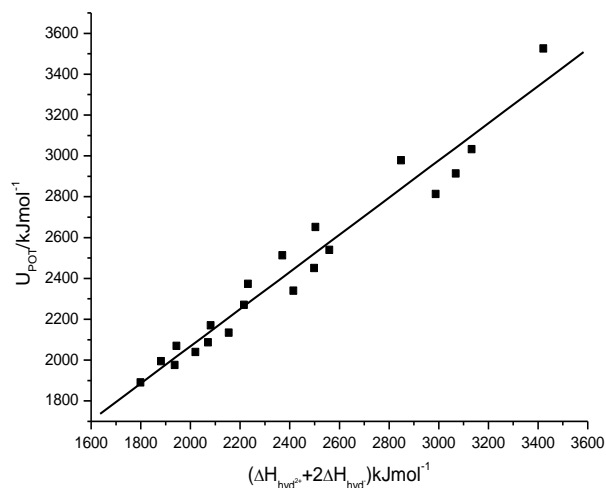


Fig. 2: Lattice energies for group 2 halides, as function of the sum of the hydration enthalpies to the respective cations and (x 2) the hydration enthalpies to the anions.

When lattice energy is plotted as a function of the sum of the respective cation and (plus 2) anion hydration enthalpies, the curve shown in Figure 2 ($r = 0.9775$) is obtained, from which the following empirical equation is derived:

$$U_{POT} = 0.909 (\Delta H_{hyd}^{2+} + 2\Delta H_{hyd}^{-}) + 248.573 \quad (4)$$

The same procedures were repeated to group some halides, and the respective data are summarized in Table 3. The experimental hydration enthalpies for trications are those provided by (Smith, 1977). In Tables 1-3, the U_{POT} values taken as references are those previously reported (Glasser, 2000; Mu, 2000).

The agreement between reference and lattice enthalpies calculated by using the equation:

$$U_{POT} = (\Delta H_{hyd}^{+} + 3\Delta H_{hyd}^{-})$$

(5)

is very good, as verified in Table 3 data.

Table.3: Hydration enthalpies (kJmol^{-1}) for some trications and group 17 monoanions, and the lattice energies (kJmol^{-1}) for the respective halides

	$-\Delta H_{hyd}^0$	$\Delta H_{hyd}^{3+} + 3\Delta H_{hyd}^{-}$	$U_{POT} \text{ (Ref.)}$	$\Delta\%$
Fe^{3+}	4430			
Al^{3+}	4665			
Ti^{3+}	4154			
Ti^{3+}	4105			
Cr^{3+}	4560			
Ga^{3+}	4700			
F^{-}	463.7			
Cl^{-}	319.5			
Br^{-}	288.7			

I	246.8			
FeCl ₃	5389	5436	-0.9	
AlF ₃	6056	6252	-3.1	
AlCl ₃	5624	5513	+2.3	
AlBr ₃	5531	5360	+3.2	
AlI ₃	5406	5227	+3.4	
TiF ₃	5545	5665	-2.1	
TiCl ₃	5113	5153	-0.8	
TiBr ₃	5020	5023	-0.1	
TiI ₃	4894	4971	-1.5	
TiF ₃	5496	5431	+1.2	
TiCl ₃	5064	5278	-4.1	
TiBr ₃	4971	5146	-3;4	
CrF ₃	5951	6065	-1.9	
CrCl ₃	5519	5529	-0.2	
CrI ₃	5300	5294	+0.1	
GaF ₃	6091	6238	-2.4	
GaCl ₃	5659	5665	-0.1	
GaBr ₃	5566	5569	-0.1	
GaI ₃	5440	5496	-1.0	

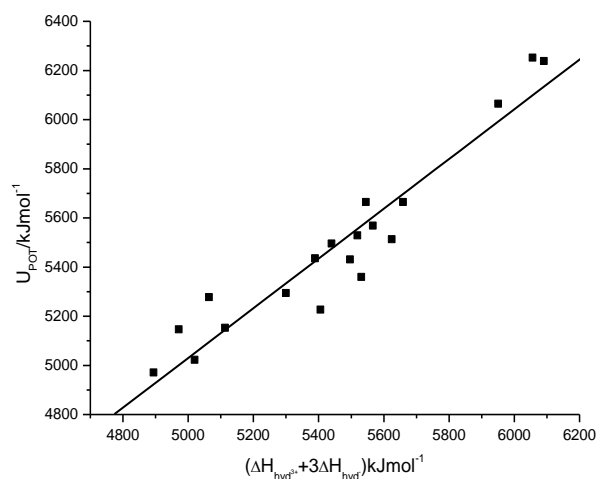


Fig. 3: Lattice energies for trication halides, as function of the sum of the hydration enthalpies to the respective cations and (x 3) the hydration enthalpies to the anions.

When lattice energy is plotted as a function of the sum of the respective cation and (x 3) anion hydration enthalpies, the curve shown in Figure 3 ($r = 0.9515$) is obtained, from which the following empirical equation is derived:

$$U_{POT} = 1.012 (\Delta H_{hyd}^{3+} + 3\Delta H_{hyd}^{-}) - 30.211 \quad (6)$$

The same procedures were repeated to some +4 cations halides, and the respective data are summarized in Table 4. The experimental hydration enthalpies for tetracations are those provided by (Smith, 1977).

The agreement between reference and lattice enthalpies calculated by using the equation:

$$U_{POT} = (\Delta H_{hyd}^{+} + 4\Delta H_{hyd}^{-}) \quad (7)$$

is very good, as verified in Table 4 data.

Table.4: Hydration enthalpies (kJmol^{-1}) for Zr^{4+} and Sn^{4+} and group 17 monoanions, and the lattice energies (kJmol^{-1}) for the respective halides.

	$-\Delta H_{hyd}^0$	$\Delta H_{hyd}^{4+} + 4\Delta H_{hyd}^{-}$	$U_{POT} \text{ (Ref.)}$	$\Delta\%$
Zr^{4+}	6953			
Sn^{4+}	7591			
F^{-}	463.7			
Cl^{-}	319.5			
Br^{-}	288.7			
I^{-}	246.8			
ZrF_4		8808	8971	-1.8
ZrCl_4		8231	8144	+1.1
ZrBr_4		8108	7984	+1.6
ZrI_4		7940	7801	-1.8
SnCl_4		8869	8930	-0.7
SnBr_4		8746	8852	-1.2

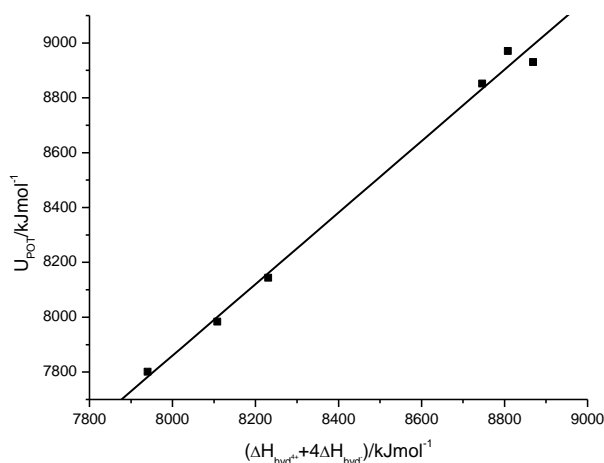


Fig. 4. Lattice energies for tetrachalcogenides, as function of the sum of the hydration enthalpies to the respective cations and (x 4) the hydration enthalpies to the anions.

When lattice energy is plotted as a function of the sum of the respective cation and (x 4) anion hydration enthalpies, the curve shown in Figure 4 ($r = 0.9969$) is obtained, from which the following empirical equation is derived:

$$U_{POT} = 1.303 (\Delta H_{hyd}^{4+} + 4\Delta H_{hyd}^{-}) - 2566.765 \quad (8)$$

Of course, Eq. (2), (4), (6) and (8) are improved versions of Eq. (1), (3), (5) and (7), and are parametrized in order to take into account factors such as dilution and entropic contributions (Persson, 2010; Hünenberger, 2011).

In order to verify the reliability and general application of Eq.(1), (3) and (5), they were employed to calculate the lattice energies for a series of salts. Despite the fact that the equations were obtained based on data for halides, they were also applied to salts with another kind of anions. The employed auxiliary data and the obtained results are summarized in Table 5. Of course, is possible to apply the values calculated by Eq.(1), (3) and (5) in Eq. (2), (4) and (6) and obtain a new set of calculated values.

Table.5: Calculated lattice energies (kJmol^{-1}) for a series of salts, employing Eq. (1), (3) or (5). The reference hydration enthalpies and lattice energies are in kJmol^{-1} .

	$-\Delta H_{hyd}^0$	U_{POT}	$U_{POT} \text{ (Ref.)}$	$\Delta\%$
		(Eq. 1, 3 or 5)		
Cu^{+}	593			
Ag^{+}	473			
Au^{+}	615			
TI^{+}	326			
F^{-}	463.7			
Cl^{-}	319.5			
Br^{-}	288.7			
I^{-}	246.8			
S^{-2}	1495			
CuF		1057	1088	-2.8
CuCl		913	996	-8.3
CuBr		882	978	-9.8
CuI		840	966	-13.0
AgF		937	974	-3.8
AgCl		793	918	-13.6
AgBr		762	905	-15.8
AgI		720	892	-19.3
AuCl		935	1066	-12.3
		(1144) ^a		(+7.3)
AuBr		904	1059	-14.6
		(1106) ^a		(+4.4)
AuI		862	1070	-19.4
		(1055) ^a		(-1.4)
TI^{I}		790	920	-14.1
		(980) ^a		(+6.5)
TI^{Cl}		646	822	-21.4
		(801) ^a		(-2.6)
TI^{Br}		615	798	-22.9
		(763) ^a		(-4.4)
TI^{I}		573	762	-24.8
		(711) ^a		(-6.7)
Cu^{2+}	2100			
Mn^{2+}	1841			
Zn^{2+}	2046			
Cd^{2+}	1807			

Ni ²⁺	2105
Co ²⁺	1996
Sn ²⁺	1556
Be ²⁺	2494
Mg ²⁺	1921
Ca ²⁺	1577
Sr ²⁺	1443
Ba ²⁺	1305

BeS	3989	3770	+5.8
MgS	3416	3238	+5.5
CaS	3072	2966	+3.6
SrS	2938	2779	+5.7
BaS	2800	2643	+5.9
CuS	3595	3694	-2.5
MnS	3336	3795	-12.0
NiS	3600	3415	+5.4
ZnS	3541	3674	-3.8
SnS	3051	3201	-4.7
CdS	3302	3460	-4.6
CoS	3491	3653	-4.4
CuF ₂	3027	3102	-2.4
CuCl ₂	2739	2824	-3.0
CuBr ₂	2677	2774	-3.5
CuI ₂	2594	2694	-3.7

MnF ₂	2768	2803	-1.2
MnCl ₂	2480	2551	-2.8
MnBr ₂	2418	2482	-2.6
MnI ₂	2335	2388	-2.2

Mn ³⁺	4544
La ³⁺	3296
Ce ³⁺	3337

MnF ₃	5935	6012	-1.3
MnCl ₃	5503	5556	-1.0
LaCl ₃	4255	4242	+0.3
LaBr ₃	4162	4280	-2.8
LaI ₃	4036	3986	+1.3
CeCl ₃	4296	4348	-1.2
CeBr ₃	4203	4418	-4.9
CeI ₃	4077	4061	+0.4

In Table 5, the experimental hydration enthalpies for cations are those provided by (Smith, 1977). Except for F⁻, Cl⁻, Br⁻ and I⁻, for which were used the values provided by Housecroft (Housecroft, 2017), the hydration enthalpies for anions are those provided by (Smith, 1977).

As can be verified from Table 5 data, Eq. (1) works very well for CuF and AgF. However, as the anion hardness decreases, the agreement between calculated and

reference values turns bad. This is a surprisingly result, since Cu⁺ and Ag⁺ are soft acids, and F⁻ is hard base. For example, when applying average orbital electronegativities to calculated lattice energies (de Farias, 2017), it was verified (in agreement with HSAB theory) that the worst results were obtained, exactly, to CuF and AgF.

On the other hand, for all copper (II) halides, Eq. (3) provides very good results. Hydrated Cu(I), d^{10} , [Cu(H₂O)₄]⁺ exhibits a tetrahedral geometry, whereas hydrated Cu(II), d^9 , [Cu(H₂O)₆]²⁺ has an octahedral structure, with Jahn-Teller distortion (Persson, 2010). The same structures (tetrahedral and octahedral) are those exhibited by Cu(I) and Cu(II) halides (Villars, 2014). Hence, for Cu(I) halides, the crystal field stabilization energy (CFSE) is zero, whereas for Cu(II) compounds, there is a net CFSE to be computed (Pfennig, 2015).

So, it is possible to suppose that Eq.(1) works better for compounds for which a zero or minor CFSE is computed (a natural conclusion, since it was obtained by using experimental data for group 1 halides).

The spectrochemical series for the halides is F⁻ > Cl⁻ > Br⁻ > I⁻ (Pfennig, 2015)., and all halides anions are weaker field ligands than water. Since, considering only the halides, F⁻ is the ligand with the strongest field, this is the explanation why to exchange four water molecules by four F⁻ ions in the coordination sphere of Cu(I) leads to a very good lattice energy calculated by using Eq. (1), whereas the results turns progressively bad for Cl⁻, Br⁻ and I⁻.

It is also necessary to consider that, despite the fact that Li⁺ is a hard acid and that Cu⁺ is a soft acid, four coordinated Li⁺ (Mähler, 2012) and four coordinated Cu⁺ (Shannon, 1976) have the same radius: 60 pm. Hence, like in Kapustinskii equation (Kapustinskii, 1956), eq.(1) is closely related with the cation radius.

Furthermore, the number of water molecules in the coordination sphere increases from Li⁺ to Cs⁺ (Persson, 2010; Mähler, 2012), and then, whereas Li⁺ is also four coordinated (like Cu⁺), Na⁺ and K⁺, for example, have six and eight water molecules in their coordination sphere (Persson, 2010; Mähler, 2012). Then, the entropic contribution is more prominent for Cu⁺ than to Cu²⁺ halides, if the lattice energies are calculated by using hydration enthalpy data.

Based on the results obtained to Ag⁺ halides (Table 5) can be concluded that Eq.(1) provides underestimated lattice energy values for compounds with a high degree of covalence, and that such disagreement (between calculated and reference values) increases as the degree of covalence increases. Since Ag⁺ is a soft acid, the degree of covalence increases from F⁻, Cl⁻ (hard bases) to Br⁻ (borderline base) and I⁻ (soft base).

For Au(I) halides the obtained results are really not good. However, Is necessary to remember that for gold, ($Z = 79$), relativistic contributions matters (Leszczynski, 2010), and that gold is the element with the (proportionally) higher relativistic contraction/effects.

The relativistic and non-relativistic equations can be related by using $\gamma = 1/[1-(v^2/c^2)]$, where v is the velocity of the considered body (in our case, an electron). The velocity of the 1s electron is $\approx Z/137$, where Z is the atomic number. Hence, $\gamma = 1/[1-((Z/137)^2/c^2)]^{1/2}$. For gold ($Z = 79$), and so, $\gamma = 1.224$.

Multiplying the lattice energy values calculated using Eq. (1), by γ , "corrected" lattice energy values are calculated for gold, and are shown between parenthesis in Table 5. Is worth noting that, considering the relativistic corrected values, the agreement between calculated and reference values increases from Cl^- to I^- , in agreement with the fact the Au^+ is a soft acid and Cl^- is a hard base, Br^- a borderline base and I^- a soft base.

A relativistic correction is also necessary for thallium halides. For Th, $Z=81$, and $\gamma = 1.240$.

As can be verified from Table 5 data, despite the fact that it was derived from group 1 halides data, Eq. (1) works well for group 2 sulfides, as well as for other +2 cations sulfides (CuS , MnS , etc.). Hence, can be concluded that Eq.(1) works for any 1:1 compounds, despite the cation or anion charge/nature.

Housecroft (Housecroft, 2017), based on hydration enthalpy data for group 1 cations and group 17 anions, have derived the following equations:

$$\Delta_{\text{hyd}} H^o = -(48.2 V_m^{-1/3} + 154.6)$$

(9)

$$\Delta_{\text{hyd}} H^o = -(214.71 V_m^{-1/3} + 271.96)$$

(10)

Eq. (9) is valid for + 1 cations and Eq. (10) is valid for -1 anions. In such equations, V_m is the cation or anion volume, a paramount parameter in volume based thermodynamics, VBT (Glasser, 2011).

Hence, Eq.(1) can be rewritten as:

$$U_{\text{POT}} = [- (48.2 V_m^{-1/3} + 154.6) - (214.71 V_m^{-1/3} + 271.96)]$$

(11)

In Eq.(11), (+) and (-) superscripts were included to differentiate between cation and anion volumes.

Furthermore, it was shown that there are a very close relationship between hydration enthalpies and absolute hardness for cations and anions. For group 1 cations (Kaya, de Farias, 2018).

$$\Delta_{\text{hyd}} H^o = -(9.645 \eta^+ + 245.930)$$

(12)

where η^+ = cation absolute hardness (eV).

For group 17 anions:

$$\Delta_{\text{hyd}} H^o = -(64.601 \eta^- + 12.321)$$

(13)

Hence, Eq.(1) can be rewritten as:

$$U_{\text{POT}} = [-(9.645 \eta^+ + 245.930) - (64.601 \eta^- + 12.321)]$$

(14)

Taking Eq. (11) and (14), and multiplying both sides by -1, we have:

$$[(48.2 V_m^{-1/3} + 154.6) + (214.71 V_m^{-1/3} + 271.96)] = [(9.645 \eta^+ + 245.930) + (64.601 \eta^- + 12.321)] ;$$

$$48.2 V_m^{-1/3} + 214.71 V_m^{-1/3} + 426.6 = 9.645 \eta^+ + 64.601 \eta^- + 258.3;$$

$$48.2 V_m^{-1/3} + 214.71 V_m^{-1/3} + 168.6 = 9.645 \eta^+ + 64.601 \eta^- ;$$

$$48.2 (V_m^{-1/3} + 4.5 V_m^{-1/3} + 3.5) = 9.645 (\eta^+ + 6.7 \eta^-);$$

$$5 (V_m^{-1/3} + 4.5 V_m^{-1/3} + 3.5) = (\eta^+ + 6.7 \eta^-);$$

$$[(V_m^{-1/3} + 4.5 V_m^{-1/3} + 3.5) / (\eta^+ + 6.7 \eta^-)] = 1/5 \quad (15)$$

Eq. (15) shows that the cation and anion volumes (obtained by X-ray data), are very closely related with the cation and anion absolute hardness, that is, are very closely relates with the frontier (homo and lomo) orbitals energies.

It is noteworthy that have been shown that (Tissander, 1998) absolute hydration enthalpy values can be calculated from a set of cluster-ion solvation data, without the use of extra thermodynamic assumptions. Hence, could be concluded that the empirical equations obtained in the present work (Eq. 15, for example), can also be related with the previously derived hydration enthalpy equations, based on cluster-pair-based approximation.

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