THE GOLDEN RATIO, ATOMIC, IONIC AND MOLECULAR CAPACITIES AND BONDING DISTANCES IN HYDRIDES

Raji Heyrovska

J. Heyrovsky Institute of Physical Chemistry,
Academy of Sciences of the Czech Republic,
182 23 Prague 8, Czech Republic.
Raji.Heyrovska@jh-inst.cas.cz

It was shown[1] recently that the ground state energy of atomic hydrogen is also the electromagnetic energy of the ***simplest atomic condenser*** consisting of an electron (e^-) and a proton (p^+) separated by the Bohr radius, a_B,

$$eI_H = e^2/2\kappa a_B = (e^2/2\kappa)[(1/a_p) - (1/a_e)] \qquad (1)$$

where I_H is the ionization potential, κ is the dielectric constant, a_B is divided into the Golden sections a_e and a_p at the point of charge neutrality, $a_e = \phi a_p = a_B/\phi$ and $\phi = \phi^2 - 1 = (1+5^{1/2})/2 = 1.618$ is the Golden ratio, $\kappa a_p = C_p$, $\kappa a_e = C_e$ are capacities of e^- and p^+ and $\kappa a_B = C_B$ is their Golden mean ***atomic capacity***. See[2] for capacity-based low level hydrogen sensors. For H as a ***Golden ellipsoid,*** with a_B as the major axis, the inter-focal distance = a_B/ϕ (= a_e).

The single bond distance between two atoms, d(AA) is[3] twice the covalent radius d(A) ***for any atom A*** and is[1] the sum of the cationic radius d(A+) and anionic radius d(A-) as shown below,

$$d(AA) = d(A+) + d(A-) = \phi^2 d(A+) = \phi d(A-) \qquad (2)$$

where ϕ divides d(AA) into the Golden sections d(A+) and d(A-) at the point of charge neutrality. The ionization potential I(AA) = $e/2\kappa d(AA)$ is given by (similar to eq. 1),

$$e/2\kappa d(AA) = (e/2\kappa)[1/d(A+) - 1/d(A-)] \qquad (3)$$

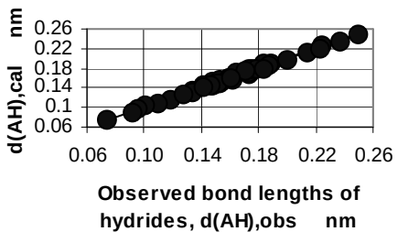
where $\kappa d(A+) = C(A+)$ and $\kappa d(A-) = C(A-)$ are ionic capacities and $\kappa d(AA) = C(AA)$ is the Golden mean ***molecular capacity*** of AA (= A_2).

On the basis of eq. 2, the inter-ionic distances d(MX) of all alkali halides (MX) were expalined[1] by the sums, d(M+) + d(X-), and hence no need for radius ratio corrections[3].

Here, the 1:1 agreement of the calculated values d(AH),cal using the data[3,4] for d(HH) and d(AA) for calculating the radii from eq. 2 with the observed[3,4] distances d(AH),obs for about 40 hydrides (***storage materials for hydrogen***), is shown in the Table and Figure in the next column. Note that some partially ionic AH bonds (like hydrogen halides) are accounted for by an ionic and a covalent bond.

Table. Comparison of d(AH),obs,[3,4] with d(AH),cal (in nm) for hydrides.

A	d(AA)/2 obs	**d(AH), obs**	d(AH),cal =	**d(AH), cal**
H	0.037	**0.074**	d(H+)+d(H-)	**0.074**
Li	0.175	**0.160**	d(A+)+d(H+)	**0.161**
Na	0.211	**0.189**	d(A+)+d(H+)	**0.189**
K	0.261	**0.224**	d(A+)+d(H+)	**0.228**
Rb	0.248	**0.237**	d(A+)+d(H-)	**0.235**
Cs	0.265	**0.249**	d(A+)+d(H-)	**0.249**
Be	0.114	**0.134**	d(A+)+d(H-)	**0.133**
Mg	0.161	**0.173**	d(A+)+d(H-)	**0.169**
Ca	0.198	**0.200**	d(A+)+d(H-)	**0.197**
Sr	0.243	**0.215**	d(A+)+d(H+)	**0.213**
Ba	0.251	**0.223**	d(A+)+d(H+)	**0.220**
Mn	0.133	**0.173**	d(A)+d(H)	**0.170**
Fe	0.144	**0.148**	d(A+)+d(H)	**0.147**
Co	0.126	**0.154**	d(A)+d(H+)	**0.154**
Ni	0.125	**0.148**	d(A)+d(H+)	**0.153**
Cu	0.128	**0.146**	d(A+)+d(H-)	**0.144**
Ag	0.144	**0.162**	d(A+)+d(H-)	**0.156**
Au	0.144	**0.152**	d(A+)+d(H-)	**0.156**
Zn	0.133	**0.160**	d(A)+d(H+)	**0.161**
Cd	0.149	**0.176**	d(A)+d(H+)	**0.177**
Hg	0.150	**0.174**	d(A)+d(H+)	**0.178**
B	0.089	**0.119**	d(A)+d(H+)	**0.117**
Al	0.143	**0.165**	d(A)+d(H+)	**0.171**
In	0.163	**0.184**	d(A)+d(H+)	**0.191**
Tl	0.194	**0.187**	d(A+)+d(H)	**0.185**
C	0.072	**0.110**	d(A)+d(H)	**0.109**
Si	0.118	**0.148**	d(A)+d(H+)	**0.146**
Ge	0.123	**0.153**	d(A)+d(H+)	**0.151**
Sn	0.151	**0.179**	d(A)+d(H+)	**0.179**
Pb	0.175	**0.184**	d(A+)+d(H-)	**0.180**
A	0.055	**0.101**	d(A-)+d(H)	**0.105**
P	0.109	**0.142**	d(A)+d(H)	**0.146**
As	0.122	**0.152**	d(A)+d(H+)	**0.150**
Sb	0.145	**0.171**	d(A)+d(H+)	**0.173**
O	0.060	**0.096**	d(A)+d(H)	**0.097**
S	0.094	**0.134**	d(A)+d(H)	**0.131**
Se	0.108	**0.147**	d(A)+d(H)	**0.145**
F	0.071	**0.092**	d(A+)+d(H)	**0.091**
Cl	0.099	**0.127**	d(A)+d(H+)	**0.127**
Br	0.115	**0.142**	d(A)+d(H+)	**0.143**
I	0.133	**0.161**	d(A)+d(H+)	**0.161**



References:
1. R. Heyrovska, 35th Mtg. of DAMOP, APS, May 2004, Tucson, AZ, abs: P1.132 & P1. 133.
2. http://www.hydrogensafety.info/articles/04-feb-08.asp
3. L. Pauling, *The Nature of the Chemical Bond*, Cornell Univ. Press, New York, 1960.
4. *CRC Handbook of C & P*, 1998 – 1999.