Spectroscopic Bond Lengths in Gaseous Alkali Halides as Sums of Bohr Radius of Alkali Metal Atoms and Covalent Radius of Halogen Atoms

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Abstract. This is a short report in support of the additivity of radii of adjacent atoms or ions in bond lengths. Here the spectroscopic bond lengths of gaseous alkali halides (MX), where M stands for alkali metals Na, K, Rb and Cs and X stands for halogens Cl, Br and I, are shown to be sums of the Bohr radii of M and covalent radii of X.

Introduction. It was recently shown [1] that bond lengths obtained by electron diffraction [2] of gaseous Na. K. Rb and Cs chlorides were close to the sum of the Golden ratio based cation radii of these alkali metals and covalent radius of Cl. It was also pointed out [1] that in the case of NaCl, the cationic radius has the same value as the Bohr radius, see the Figures in [3]. The spectroscopic values for bond lengths in [4] are slightly less than those reported in [2]. These data [4] have been used to show here that the bond lengths of gaseous halides (MX) of the above alkali metals (M) with X = Cl, Br and I are sums of the relevant Bohr radii a_B of the alkali metals (M) and the covalent radii of the halogens (X).

Data and interpretation. The spectroscopic observed bond lengths $d(MX)_{obs}$ tabulated by NIST [4] of gaseous alkali halides (MX) listed in col 1 of Table 1 are given (in A) in col 2. The Bohr radii a_B (M) of the alkali metals calculated [3] from the first ionization potentials are tabulated in

col. 3. The covalent radii $R(X)_{cov}$ of the halogens from [3, 5] are in col. 4. The sums d(MX),cal

of the radii in cols 3 and 4 are given in col 5. The last column in the Table gives the difference

between the observed and calculated radii.

Table 1. Bond lengths of gaseous alkali halides.

col.nr. 1	2	3	4	5	6
MX	d(MX),obs	a(B),M	R(X),cov	d(MX),cal	d(cal-obs)
				cols (3+4)	cols (5-2)
NaCl	2.361	1.40	0.99	2.39	0.03
KCl	2.667	1.66	0.99	2.65	-0.02
RbCl	2.787	1.72	0.99	2.71	-0.08
CsCl	2.906	1.85	0.99	2.84	-0.07
NaBr	2.502	1.40	1.15	2.55	0.05
KBr	2.821	1.66	1.15	2.81	-0.01
RbBr	2.945	1.72	1.15	2.87	0.08
CsBr	3.072	1.85	1.15	3.00	-0.07
NaI	2.711	1.40	1.33	2.73	0.02
KI	3.048	1.66	1.33	2.99	-0.06
RbI	3.177	1.72	1.33	3.05	-0.13
CsI	3.315	1.85	1.33	3.18	-0.14

It can be seen that the difference is less than +/- 0.1 A. The gaseous bond lengths obtained by

spectroscopy are thus sums of the Bohr radii of the alkali metals and the covalent radii of the

halogens which are non-ionic. The values obtained by electron diffraction [2], on the other hand,

are slightly higher [1] and are sums of the Golden ratio based metal ion radii and covalent radii

of halogens, see [3] for figures of the various radii of the atoms and ions.

References

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