Approximate sizes of monoatomic negative ions with fractional nuclear charge using electrostatic potentials

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Summary. Using the criterion that for negative monoatomic ions with N electrons, the location of minimum in the electrostatic potential $V(r)$ gives an approximate estimate of ionic radii, r_m. Calculations of the latter are reported for quark atoms with fractional nuclear charges $Z = N - \frac{1}{3}$ and $N - \frac{2}{3}$, respectively. Quark atoms with $N = 1$–10, 18 and 36 have also been considered.

1. Introduction

Lackner and Zweig [1] have discussed the importance of electronegativity and crystal radii, respectively, in predicting the chemistry of quark atoms. Quark atoms are defined as having integral numbers of electron (N) but nuclear charges (Z) that differ by $\pm\frac{1}{3}$ or $\pm\frac{2}{3}$ from integral values. Sen et al. [2] have recently studied the isoelectronic energy and electronegativity differences of quark atoms. Quark atoms are always ionic species, since for $Z \neq N$. The purpose of this paper is to report the results of our calculations of approximate ionic radii, r_m, corresponding to the negatively charged quark atoms defined by $Z = N - \frac{1}{3}$ and $N - \frac{2}{3}$, respectively. In particular, we have considered atoms with $N = 1$–10, 18 and 36 respectively.

2. Method of calculation

The calculations of r_m have been carried out using the method described by Sen and Politzer [3]. In brief, r_m corresponds to the minimum in the electrostatic potential, $V(r)$, of the mononegative atom. The quantity $V(r)$ is rigorously given by

$$V(r) = \frac{Z}{r} - \int \frac{\varrho(r')}{|r' - r|} \, dr' \tag{1}$$

Within the spherical approximation, imposing the condition $dV(r)/dr = 0$ on Eq.

(1) leads to the following criterion for calculating r_m.

$$Z = 4\pi \int_0^{r_m} r'^2 \varrho(r') \, dr' \qquad (2)$$

Sen and Politzer [3] have shown that r_m can be interpreted as the crystal ionic radii of mononegative ions in a homogeneous crystal. In order to calculate r_m, we have computed $\varrho(r)$ by means of a quasirelativistic self-consistent field local spin density functional approximation [4] including the self interaction correction and correlation effects. Appropriate fractional nuclear charges have been used through the calculations. A detailed account of the numerical methods adopted by us has been described earlier [2, 4].

3. Results and conclusions

In order to test the reliability of the calculated values of r_m, in Table 1 our previous [3] theoretical values for halogen and alkali metal negative ions are compared with the recent experimental estimates [5]. The two sets of values are found to be in good agreement.

In Table 2, the theoretical values calculated in this work for the ionic radii of the quark atoms with $Z = N - \frac{1}{3}$ and $N - \frac{2}{3}$ are presented. The corresponding theoretical r_m values of the ordinary mononegative atoms ($Z = N - 1$) are also given [3]. For all atoms except hydrogen, the ionic radius corresponding to $Z = N - \frac{2}{3}$ is found to be smaller than that of $Z = N - \frac{1}{3}$. This counter-intuitive trend could be understood in terms of Eq. (2). The integrated charge density, Eq. (2), attains the value $Z = (N - \frac{2}{3})$ at a smaller radial distance than the value $N - \frac{1}{3}$. However, for hydrogen ($Z = \frac{1}{3}$), the electronic charge ($N = 1$) is three times the nuclear charge. This condition corresponds to an unusually diffuse charge distribution and the integrated charge density attains the value of $\frac{1}{3}$ at a higher r_m than that corresponding to the $N = Z - \frac{1}{3}$ case. We note here that our

Table 1. A comparison of theoretical values of ionic radii for halogen and alkali metal negative ions with the experimental values. All values are in Å

	Theoretical[a]	Experimental
F⁻	1.08	1.15[b]
Cl⁻	1.63	1.67[b]
Br⁻	1.79	1.82[b]
I⁻	2.05	2.06[b]
Na⁻	2.69	2.77[c]
K⁻	3.19	3.30[c]
Rb⁻	3.33	3.37[c]
Cs⁻	3.53	3.60[c]

[a] Ref. [2]
[b] Shanon RD (1976) Acta Cryst Sect A 32:751. Crystal radii on page 760
[c] Huang RH, Ward DL, Dye JL (1989) J Am Chem Soc 111:5707, Table II, Column 6

Table 2. Theoretical estimate of approximate ionic radii (Å) for quark atoms with $Z = N - \frac{1}{3}$ and $N - \frac{2}{3}$, respectively. The entries in last column correspond to the ordinary mononegative atoms in their ground state

Atom	N	Z		
		$N - \frac{1}{3}$	$N - \frac{2}{3}$	$N - 1$
H	1	1.39	1.65	a
He	2	0.98	0.96	1.11(H^-)
Li	3	2.88	2.31	b
Be	4	2.34	2.36	2.59(Li^-)
B	5	2.07	2.01	2.22(C^-)
C	6	1.77	1.72	1.76(B^-)
N	7	1.56	1.47	1.48(Be^-)
O	8	1.42	1.34	1.34(N^-)
F	9	1.30	1.22	1.19(O^-)
Ne	10	1.21	1.12	1.08(F^-)
Ar	18	1.78	1.67	1.63(Cl^-)
Kr	36	1.96	1.84	1.79(Br^-)

[a] At $Z = 0.1$, for $N = 1$, $r_m = 2.86$ Å
[b] No convergence

calculated value of 1.39 Å for the ionic radius of H $(Z = N - \frac{1}{3})$ is in good agreement with the estimated crystal radius of 1.50 Å of Lackner and Zweig [6].

We hope that the present calculations of ionic radii will be useful in the design of experiments to search for quarks.

References

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