TABLE II

Ionic radii (in Angstroms) in the alkali halides at atmospheric pressure

	F^-		Cl^-		Br^-		I^-
Li^+	0·727	1·271	0·760	1·800	0·770	1·990	0·786	2·270
Na^+	1·066	1·259	1·105	1·706	1·111	1·849	1·144	2·114
K^+	1·425	1·272	1·457	1·688	1·461	1·826	1·481	2·040
Rb^+	1·563	1·255	1·598	1·693	1·610	1·851	1·611	2·025
Cs^+	1·766	1·230	1·844	1·752	1·845	1·886	1·846	2·060

Tosi and Fumi[4] are 1·381% for r and 6·06% for d^2W_i/dr^2.

In earlier papers[2,3] we claimed that the r.m.s. fit in r and d^2W_i/dr^2 obtained with our potentials is superior to that obtained with the potentials of Tosi and Fumi[4]. This claim is not correct since the r.m.s. errors (for the potentials of Tosi and Fumi) 1·435% and 15·40% quoted there arose from a computational error. The present comparison indicates that the fit in the two theories are of the same order. However, the advantages of the present formulation mentioned at the beginning of this paper are still valid.

The repulsion parameters listed in Table I are different from those listed in references 2 and 3. However, the ionic radii (listed in Table II) predicted by the new set of parameters are not significantly different. During the refinement, the radii of the ions remained almost the same while the compressibility of the ions, which is qualitatively measured by the parameter ρ, varied considerably. The essential difference of the present set of repulsion parameters from the earlier set[2,3] is that the alkali ions are much harder and the halogen ions much softer than predicted by the earlier parameters.

As a consequence, the present repulsion parameters indicate that the alkali ions are much less compressible than the halogen ions. For instance, calculations show that in CsI, between 0 and 40 kbars, the radius of Cs^+ decreases by 0·062 Å while the radius of I^- decreases by 0·159 Å. In LiF, between 0 and 150 kbars, the radius of Li^+ decreases by only 0·017 Å while the radius of F^- decreases by only 0·017 Å while the radius of F^- consistent with the relatively large polarizabilities of the halogen ions. The compressibilities of ions will be discussed in some detail in a later communication.

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