Review: Chapter 18-Nature of the Ionic Bond of Alkali Hydrides

Mark W. Nansteel, January 23, 2007

Synopsis

The structure of six alkali hydrides are studied. The bond length between the metal and hydrogen ions and the energy of the crystal lattice are calculated using principles of electrostatics, previously calculated ionic radii, and bond energies of the alkali metals. In all, five normal hydrides and one hydrino hydride are considered: lithium hydride (LiH), sodium hydride (NaH), potassium hydride (KH), rubidium hydride (RbH), cesium hydride (CsH), potassium hydrino hydride (KH(1/4)). In calculating the lattice energy the Madelung constant appropriate for the face-centered NaCl-like structures is used to account for the electrostatic force on a given ion due to the system of ions in the lattice. The calculated inter-ion distances and the lattice energies are compared with experimental data for all five normal hydrides. The agreement between the theory and measured values is very good, especially considering the uncertainty in the measurements. The mean variation of the calculated and experimental inter-ion distance is 1.8% (ignoring LiH for which the experimental measurement uncertainty is particularly large) and the corresponding variation is 1.1% for the lattice energy. The table below lists the inter-ion distances, r_0, and lattice energies, ΔU, along with the computed percent variance of the theory from the measurements.

Comparison of experimental and calculated inter-ion distance and lattice energy.

	$r_0 \times 10^{10}$ [m]	$r_0 \times 10^{10}$ (calculated) [m]	Δ(%)	ΔU [kcal/mol]	ΔU (calculated) [kcal/mol]	Δ(%)
LiH	2.04	2.34	14.7	218.0	217.8	0.1
NaH	2.44	2.45	0.4	202.0	206.6	2.2
KH	2.85	2.83	0.7	177.2	174.3	1.6
RbH	3.02	2.92	3.3	168.6	168.3	0.2
CsH	3.19	3.10	2.8	154.5	156.9	1.6

Equation verification

The equations in Chapter 18 were checked for internal (internal to Chapter 18) algebraic and dimensional consistency, numerical accuracy, and clarity of presentation. All of the numerical results were verified by hand calculation. The following set of numerical constants was used in the verification process:

$$e = 1.6022 \times 10^{-19} \text{ C}$$
$$\varepsilon_0 = 8.85419 \times 10^{-12} \text{ C}^2/\text{N-m}^2$$
$$M_c = 1.74756$$
$$N = 6.02214 \times 10^{23} \text{ mol}^{-1}$$