Review: Chapter 19-The Nature of the Metallic Bond of Alkali Metals

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Synopsis

The lattice structure and bond energy of the alkali metals Li, Na, K, Rb, and Cs are calculated. The metals are modeled as a two dimensional layer of charge, corresponding to the free electrons, which is bound to the lattice of positive metal ions. The separation distance between the metal ions and the electron layer, d, and the lattice constant, a, are determined by a force balance between electrostatic, magnetic, and centrifugal forces. In the cases of Cs and Rb experimental values for the lattice parameter are used to calculate the separation distance. The bond energy, E_D, is determined as the sum of electric potential, kinetic, and binding energies. The calculated lattice parameters and bond energies are compared with published experimental data for these parameters and good agreement is found. The table below lists the calculated and experimental parameters. The mean variation of the calculated and experimental lattice parameter is 1.3% and the corresponding variation is 2.2% for the lattice energy.

Comparison of experimental and calculated lattice parameter a and energy E_D.

	a x 10^{10} [m]	a x 10^{10} (calculated) [m]	Δ(%)	E_D [kJ/mol]	E_D (calculated) [kJ/mol]	Δ(%)
Li	3.51	3.61	2.8	159.3	167.8	5.3
Na	4.29	4.32	0.7	107.5	107.1	0.4
K	5.32	5.34	0.4	89	90.4	1.6
Rb				80.9	79.06	2.3
Cs				76.5	77.46	1.3

Equation verification

The equations in Chapter 19 were checked for internal (internal to Chapter 19) 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:

$$a_0 = 5.29177 \times 10^{-11} \text{ m}$$
$$e = 1.60218 \times 10^{-19} \text{ C}$$
$$\varepsilon_0 = 8.85419 \times 10^{-12} \text{ C}^2/\text{N-m}^2$$
$$\hbar = 1.05457 \times 10^{-34} \text{ J-s}$$
$$m_e = 9.1093897 \times 10^{-31} \text{ kg}$$
$$N = 6.02214 \times 10^{23} \text{ mol}^{-1}$$