

Table 2. Evaluation of A and the parameters at the minimum in the Zn curve

Metal	P_{\min} (kg/cm ²)	v_{\min} (cm ³)	$A \times 10^6$	ϕ_{\min}	Zw_{\min} <i>exact to 10 digits</i>
Lithium	84,819.8*	1.303580*	0.272219*	0.767118*	1
Sodium	55,284.8	0.711600	0.549218	1.405284	1
Potassium	16,239.1	0.865777	0.645614	1.155032	1
Rubidium	16,807.0	0.479612	1.258094	2.085020	1
Cesium low pressure	17,608.1	0.362564	6.203762	2.758131	1

* These values are truncated values from the computation in which 20 digits were used.

(3) One can interpolate in a table of P/v vs. P the value of L/J using Lagrangian interpolation.

All these computational methods have been tried. The test of the precision of the answer is to calculate Zw which should be equal to 1. The methods in 1 are computationally difficult since obtaining the logarithm to a sufficient number of digits is difficult. Method 2 is inherently imprecise, although by this method very good preliminary results were obtained, the calculation of Zw showed that they were imprecise. We used method 3 which is very precise. The results are reported in Table 2.

ATOMIC RADII

Since we now know B , for the alkali metals many other quantities become accessible to calculation. One of these is the atomic radius. B is the excluded volume of the metal, i.e. it is the volume of the associated particles in the metal. These particles may be considered to be composed of spherical atoms packed in a particular array. In the alkali metals this array is b.c.c. This configuration in addition to the atoms also has internal free space; we will call this space the internal volume of the particles. We now differentiate between the total volume, v ; the defect volume, $(v-B)$, which is the volume between particles, the excluded volume, B ; and finally the internal volume which is the space in B not occupied by the spherical atoms. To obtain the atomic radii we must first evaluate how much of the excluded volume is the internal volume.

In a body-centered array, the atoms conceived as spherical balls are touching along the diagonal

of the unit cell. Hence in terms of the radius, r , of the atom the length, l , of the unit cell is

$$(4r)^2 = 3l^2$$

or

$$l = \frac{4}{\sqrt{3}}r$$

since four atomic radii lie along the unit cell diagonal. The volume of the unit cell is then

$$l^3 = \frac{64}{3\sqrt{3}}r^3$$

Since for body-centered packing each unit cell has two atoms the volume per atom is

$$\text{volume per atom} = \frac{32}{3\sqrt{3}}r^3$$

The volume per Avogadro number of atoms (formole) is

$$\text{vol/formole} = \frac{32}{3\sqrt{3}}r^3N_0$$

Also since B is the excluded volume per gram, BM^0 is the excluded volume per formole where M^0 is the molecular weight (here at. wt.). Hence

$$BM^0 = \frac{32}{3\sqrt{3}}r^3N_0$$

solving for r we have for a b.c.c. array

$$r = \left(\frac{3\sqrt{3}}{32N_0} BM^0 \right)^{1/3} \quad (16)$$

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