

known geometrical array of individual atoms—all noble gases (except the special case of He) crystallize in the face centered cubic lattice (space group — $O_h^5$  or  $Fm\bar{3}m$ )—with weak van der Waals forces holding the lattice together. The equation of state of frozen Ne, Ar, Kr and Xe was developed already twenty years ago by KANE.<sup>(10)</sup> Recently, the quantum mechanical variational method was applied to an Einstein model of a solid and the equation of state of the same solid gases developed by

TABLE 1.—SELECTED VALUES OF THE ATOMIC CONSTANTS OF THE SOLID NOBLE GASES, ALL AT 0°K

Metal	$D_0$ , °K. (g/cm <sup>3</sup> )	Lit.	At.wt. <sup>12</sup> C = 12.0000	$V_{at}^{0°K}$ , (cm <sup>3</sup> /g atom)	$v_0$ (Å <sup>3</sup> /atom)	$a_0$ (Å)	$d_0$ (Å)	Crystal System	Atoms/ cell	Space Group
Ne	1.544	13	20.183	13.07	21.70	4.427	3.131	f.c.c.	4	$O_h^5$
Ar	1.827	13	39.948	21.86	36.29	5.255	3.716	f.c.c.	4	$O_h^5$
Kr	3.093	14	83.80	27.09	44.96	5.645	3.991	f.c.c.	4	$O_h^5$
Xe	3.783	15	131.30	34.71	57.60	6.131	4.335	f.c.c.	4	$O_h^5$
Em	(5.25)		222.0	(42.3)	(70.2)	(6.50)	(4.63)	(f.c.c.)	(4)	( $O_h^5$ )

TABLE 2.—BERNARDES<sup>(11)</sup> SELECTION OF NOBLE GAS CONSTANTS

Metal	$V_{at@}$ 0°K (cm <sup>3</sup> /g atom)	Heat of Sublimation at 0°K (cal/g atom)
Ne	13.1	420
Ar	22.6	1852
Kr	27.5	2630
Xe	35.1	3824

BERNARDES.<sup>(11)</sup> The change of volume with pressure and the compressibility follow directly from the two-body potential parameters ( $\sigma$  and  $\epsilon$ ), which are selected to give the best fit with the experimental atomic volume and heat of sublimation, both at 0°K (see Tables 1 and 2). The theoretical deviation of quantum mechanical laws of corresponding states from classical behaviour for the various properties, including compressibility, of the solid noble gases at 0°K was also determined recently by BERNARDES.<sup>(12)</sup>

The most precise lattice parameters of solid neon and argon at 4.2°K were determined by neutron diffraction by HENSHAW<sup>(13)</sup> and those of krypton<sup>(14)</sup> and xenon<sup>(15)</sup> by SMITH from X-ray data at 20° to 120°K.

The values selected by us are correlated in Table 1. It should be clarified here that the inorganic chemist is used to compare atomic volumes,  $V_{at}$ , in cm<sup>3</sup>/g atom, defined as at. wt./density,  $D$ , in g/cm<sup>3</sup>, while the crystallographer uses the dimensions and angles of a unit cell. The physicist thinks of the same properties in units of

<sup>(10)</sup> G. KANE, *Phys. Rev.*, **7**, 603–613 (1939); see also J. O. HIRSCHFELDER, C. I. CURTIS and R. B. BIRD, *Molecular Theory of Gases and Liquids*, pp. 1035–1044. J. Wiley, New York (1954).

<sup>(11)</sup> N. BERNARDES, *Phys. Rev.* **112**, 1534–39 (1958).

<sup>(12)</sup> N. BERNARDES, *Phys. Rev.* **120**, 807–813 (1960).

<sup>(13)</sup> D. G. HENSHAW, *Phys. Rev.* **111**, 1470–1475 (1958).

<sup>(14)</sup> B. F. FIGGINS and B. L. SMITH, *Phil. Mag.* [8] **5**, 186–8 (1960).

<sup>(15)</sup> A. J. EATWELL and B. L. SMITH, *Phil. Mag.* [8] **6**, 461–3 (1961).