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Densities of the alkali halides, the chalcogenides and some Cu^- Ag^- and Tl^- Halides from the nearest neighbour distance

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ABSTRACT

Nearest neighbour distances in almost all the familiar crystals have been determined from X-ray measurements which are supposed to be very accurate. These are used for the alkali halides, the chalcogenides and some Cu^-, Ag^- and Tl^- halides to calculate the molar volume. The molecular weight, taken in grams, is divided by the molar volume, to obtain the densities of these compounds in gm /cc. These densities have been given for all the alkali halides, the chalcogenides and some Cu^-, Ag^- and Tl^- halides. These densities, presented here, are expected to be more accurate than the values obtained by the conventional methods. In this light, use of the densities presented here should find wide acceptance for accurate work. Significant difference between the present values and those given in the standard literature exist only for a few cases. Both the sets of densities are given in the tables. However, small differences can be expected. The user will have to carefully decide which set is more appropriate for him. One may worry about the accuracy if there is a relatively large difference. Such cases are not too many.

Key words : Density, nearest neighbour distance, alkali halides, chalcogenides, Cu^-, Ag^- and Tl^- halides.

INTRODUCTION

Accurate data for the nearest neighbour distance r_o in most familiar crystals, including those considered here, are available in the standard literature[1-3]. These may be used to find the molar volume V_o by the well known formula

$$V_o = N K r^3_o \qquad ...(1)$$

where N is the Avagadro's number and K is a constant for a given family of compounds. The values of K for various crystal types are given in most text books of advanced inorganic chemistry. The value of K is given above the table of the concerned family. By definition, the density D is given by

$$D = \frac{M}{V_o} \qquad ...(2)$$

where M is the molecular weight, taken in gms.

RESULTS AND DISCUSSION

The densities are calculated using formulae (1) and (2). These are given in the tables 1(a) , 1(b), 2(a) 2(b), 2(c) , 2 (d) , 3 (a) , 3(b) and 3 (c), where apart from the serial number, the first column gives the name of the compound, the second column the molecular weight, calculated from the relevant atomic weights[4], the third column gives the experimental r_o , the fourth column the present densities and the last column the densities given in the standard literature[5].

Table - 1 (a): Alkali halides, NaCl type (K = 2)

S. No.	Compound	Molecular Weight M (in gms)	r_o (in Å)	Density (in gms/cc) Present work	Density (in gms/cc) from ref. 5
1.	LiF	25.93	2.013	2.646	2.64
2.	LiCl	42.39	2.570	2.078	2.07
3.	LiBr	86.85	2.751	3.460	3.464
4.	LiI	133.84	3.006	4.093	4.06
5.	NaF	41.98	2.317	2.799	2.78
6.	NaCl	58.44	2.820	2.164	2.17
7.	NaBr	102.90	2.989	3.196	3.20
8.	NaI	149.89	3.236	3.674	3.67
9.	KF	58.10	2.674	2.526	2.48
10.	KCl	74.56	3.146	1.988	1.988
11.	KBr	119.01	3.300	2.748	2.74
12.	KI	166.01	3.533	3.126	3.12
13.	RbF	104.46	2.826	3.840	3.20
14.	RbCl	120.92	3.291	2.819	2.76
15.	RbBr	165.38	3.445	3.355	3.35
16.	RbI	212.37	3.671	3.563	3.55
17.	CsF	151.90	3.004	4.645	4.64

Table - 1(b): Alkali halides CsCl type (K = 1.54)

S. No.	Compound	Molecular Weight M (in gms)	r_o (in Å)	Density (in gms/cc) Present work	Density (in gms/cc) from ref. 5
1.	CsCl	168.36	3.571	3.99	3.988
2.	CsBr	212.81	3.720	4.461	4.43
3.	CsI	259.81	3.956	4.526	4.51

Table - 2(a): Chalcogenides (Oxides) , NaCl type (K = 2)

S. No.	Compound	Molecular Weight M (in gms)	r_o (in Å)	Density (in gms/cc) Present work	Density (in gms/cc) from ref. 5
1.	MgO	40.31	2.105	3.599	3.60
2.	CaO	56.08	2.405	3.338	3.34
3.	TiO	63.90	2.090	5.809	4.95
4.	MnO	70.94	2.225	5.334	5.37
5.	FeO	71.85	2.147	6.038	6.00
6.	CoO	74.93	2.135	6.404	6.44
7.	NiO	74.71	2.085	6.854	6.72
8.	SrO	103.62	2.580	5.006	5.10
9.	NbO	108.91	2.105	9.724	7.30
10.	CdO	128.4	2.350	8.231	8.15
11.	BaO	153.34	2.760	6.061	5.72

Table - 2(b): Chalcogenides (Sulphides), NaCl type (K = 2)

S. No.	Compound	Molecular Weight M (in gms)	r_o (in Å)	Density (in gms/cc) Present work	Density (in gms/cc) from ref. 5
1.	MgS	56.38	2.540	2.862	2.68
2.	CaS	72.14	2.845	2.604	2.59
3.	MnS	87.00	2.610	4.065	4.00
4.	SrS	119.68	2.940	3.911	3.70
5.	BaS	169.40	3.195	4.310	4.30
6.	LaS	170.97	2.920	5.699	5.61
7.	CeS	172.18	2.890	5.917	5.90
8.	PbS	239.25	2.970	7.571	7.60

Table - 2(c): Chalcogenides (Selenides) , NaCl type (K = 2)

S. No.	Compound	Molecular Weight M (in gms)	r_o (in Å)	Density (in gms/cc) Present work	Density (in gms/cc) from ref. 5
1.	MgSe	103.27	2.725	4.232	4.20
2.	CaSe	119.04	2.955	3.828	3.80
3.	MnSe	133.90	2.725	5.488	5.45
4.	SrSe	166.58	3.115	4.576	4.54
5.	SnSe	197.65	3.010	6.008	6.18
6.	BaSe	216.30	3.300	4.995	5.02
7.	PbSe	286.15	3.040	8.466	8.10

Table - 2(d): Chalcogenides (Tellurides) , NaCl type (K = 2)

S. No.	Compound	Molecular Weight M (in gms)	r_o (in Å)	Density (in gms/cc) Present work	Density (in gms/cc) from ref. 5
1.	CaTe	167.68	3.170	4.367	4.87
2.	SrTe	215.22	3.330	4.836	4.83
3.	SnTe	246.29	3.155	6.516	6.50
4.	PbTe	334.79	3.225	8.287	8.164

Table - 3(a): Silver and Copper halides, ZnS – type (K = 3.08)

S. No.	Compound	Molecular Weight M (in gms)	r_o (in Å)	Density (in gms/cc) Present work	Density (in gms/cc) from ref. 5
1.	AgI	234.77	2.80	5.768	5.68
2.	CuCl	98.99	2.35	4.110	4.14
3.	CuBr	143.45	2.46	5.197	4.98
4.	CuI	190.44	2.62	5.702	5.67

Table - 3(b): Silver halides , NaCl type (K = 2)

S. No.	Compound	Molecular Weight M (in gms)	r_o (in Å)	Density (in gms/cc) Present work	Density (in gms/cc) from ref. 5
1.	AgCl	143.32	2.77	5.598	5.56
2.	AgBr	187.78	2.89	6.453	6.47

Table - 3(c): Thallous halides , CsCl type (K = 1.54)

S. No.	Compound	Molecular Weight M (in gms)	r_o (in Å)	Density (in gms/cc) Present work	Density (in gms/cc) from ref. 5
1.	Tl Cl	239.82	3.31	7.138	7.00
2.	Tl Br	284.28	3.44	7.521	7.50
3.	Tl I	331.27	3.65	7.345	7.10

RbF , TiO, NbO, BaO, MgS, SrS, SnSe, PbSe and CaTe show the greatest discrepancies. These cases may be looked into. On account of the high accuracy of the r_o, it is expected that the densities, as given here, would be widely used for accurate work. However, for obvious reasons, different methods of measurement of densities may not be expected to give exactly coincident values, but large differences are not acceptable. Small temperature differences are not expected to alter the densities significantly.

In principle, the same approach may be applicable to molecular crystals, but in many of these, there are molecular aggregates with the same number of the molecules forming each aggregated cluster that occupies each of the lattice sites of the molecular crystal. In these cases, the reverse process of using the observed density to find out the number of molecules in the cluster is more useful. More accurate density could then be predicted. Thus as an example, X-ray studies tell that the HgClBr crystal is orthorhomibic and give numerical values of the three sides. Then, using the experimental density, it was found out that clusters of eight HgClBr molecules sit on each lattice site[6]. Agglomeration does not take place in highly ionic compounds.

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