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Relationship between the unit-cell volumes and cation radii of isostructural compounds and the additivity of the molecular volumes of carbonates

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ABSTRACT

Both theoretical relations and observed structure data imply the following relationships: for a series of multi-cation isostructural compounds such as $A_mB_n \cdots Xp$, the unit-cell volume V and the radius r_A of a cation A are related, when the anion and other cations are fixed, as follows:

$$V = (p + qr_A)(r_x + r_A)^3 \qquad (p, q = \text{const.}).$$

A simplified relation for binary isostructural compounds is:

$$V = k(r_X + r_A)^3 \qquad (k = \text{const.}).$$

An approximation based on the above equations results in a linear relationship between V and r_A^3. Another approximation gives rise to a linear correlation between V and r_A. An application of the latter relationship shows that the effect of two or more cations in a multi-cation carbonate is equivalent to that of one cation whose radius is an average of the two. This implies that the molecular volume of a multi-cation carbonate is equal to the sum of the molecular volumes of the corresponding component simple carbonates. When the coordinations of cations are the same as in the simple carbonates, the additivity relation gives rise to very accurate values. Regardless of the coordinations, the molecular volume may still be obtained by addition of component volumes, though with slightly lower accuracy.

INTRODUCTION

The effective ionic radii proposed by Shannon and Prewitt (1969) are widely used in crystal chemal relations. Shannon and Prewitt (S-P) discovered the surprising result that the unit-cell volume V appears to be linearly correlated with the cube of the cation radius r^3 for a series of isostructural compounds. Furthermore, many of the S-P ionic radii were derived assuming this linearity, the significance of which was discussed by Prewitt (1985). The linear relation can be used to test the accuracy of unit-cell parameters and to predict the formation of new compounds, the volume relations attendant to solid solutions, the electron spin states of transition-metal cations and, when structural data are not available, the ionic radii. The basis for the linearity has not been discussed, however, and the relationship remains an empirical one. Hazen and Finger (1982) correctly noticed the curvature in the case of NaCl-type compounds. Indeed, apparent curves instead of straight lines occur in some cases and the reason for this is not clear. Because of such questions it is worthwhile to develop further insight into the correlation between the unit-cell volume and cation radii of isostructural compounds.

RELATIONSHIP FOR MULTI-CATION COMPOUNDS

Consider a series of ternary isostructural compounds $A_mB_nX_p$. Figure 1 shows a hypothetical unit cell of $A_mB_nX_p$. If the origin is set at a specific atom such as A, there is always at least one chain, composed of a number of bonds A-X and/or B-X, along which it is possible to proceed from the origin O(0,0,0) to E(1,1,1). The projections of the chain on the three axes are **a**, **b**, and **c**, respectively. Each is equal to the sum of the projections of the component bonds on a specific axis. A bond distance equals the sum of the radii of the cation and anion. The unit-cell edges can then be written as:

$$a = \sum_i (r_X + r_A)\cos\alpha_i + \sum_j (r_X + r_B)\cos\alpha_j \qquad (1)$$

$$b = \sum_i (r_X + r_A)\cos\beta_i + \sum_j (r_X + r_B)\cos\beta_j \qquad (2)$$

$$c = \sum_i (r_X + r_A)\cos\gamma_i + \sum_j (r_X + r_B)\cos\gamma_j \qquad (3)$$

where $r_X + r_A$ and $r_X + r_B$ are the bond distances of bonds

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X-A and X-B, respectively; α_i, β_i, γ_i are the included angles of the ith X-A bond with **a**, **b**, **c**, respectively; and α_j, β_j, γ_j are the included angles of the jth X-B bond with **a**, **b**, **c**, respectively.

The unit-cell volume can be calculated from the cell edges obtained from Equations 1–3. Assume the bond distance of X-B is t times that of X-A, then $r_X + r_B = t(r_X + r_A)$. Substituting into Equations 1–3 gives the relations:

$$a = \sum_i (r_X + r_A)\cos\alpha_i + \sum_j t(r_X + r_A)\cos\alpha_j$$

$$= (r_X + r_A)\left(\sum_i \cos\alpha_i + t\sum_j \cos\alpha_j\right)$$

$$b = \sum_i (r_X + r_A)\cos\beta_i + \sum_j t(r_X + r_A)\cos\beta_j$$

$$= (r_X + r_A)\left(\sum_i \cos\beta_i + t\sum_j \cos\beta_j\right)$$

$$c = \sum_i (r_X + r_A)\cos\gamma_i + \sum_j t(r_X + r_A)\cos\gamma_j$$

$$= (r_X + r_A)\left(\sum_i \cos\gamma_i + t\sum_j \cos\gamma_j\right).$$

Then the volume of a rectangular unit-cell is:

$$V = abc = (r_X + r_A)^3\left(\sum_i \cos\alpha_i + t\sum_j \cos\alpha_j\right) \cdot\left(\sum_i \cos\beta_i + t\sum_j \cos\beta_j\right) \cdot\left(\sum_i \cos\gamma_i + t\sum_j \cos\gamma_j\right) \quad (4)$$

When the anion X and cation B are defined, r_A is the only variable for isostructural compounds $A_mB_nX_p$. It can be reasonably assumed that the included angles α_i, β_i, γ_i, and so on are functions of r_A. Obviously, t is also a function of r_A, so the product of the terms after $(r_X + r_A)^3$ in Equation 4 is a function of r_A. The volume of a rectangular cell can then be written as:

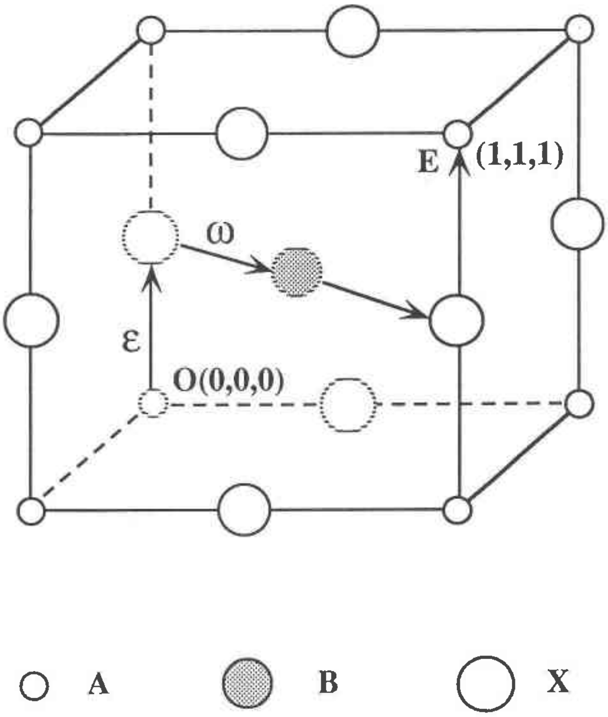

Fig. 1. A sketch of a hypothetical unit cell. The chain of bonds proceeds along the arrows from O(0,0,0) to E(1,1,1). Its projections on the three axes are **a**, **b**, and **c**, respectively.

$$V = f(r_A)(r_X + r_A)^3 \quad (5)$$

For a nonrectangular unit-cell, the axial angles are also functions of r_A. The unit-cell volume is in the same form as Equation 5.

Suppose $f(r_A)$ has derivatives of orders up to n; according to Taylor's formula, we get:

TABLE 1. Relationship between the ratio $V/(r_O + r_A)^3$ and r_A of ternary isostructural compounds

Compound	r_A	$V/(r_O + r_A)^3$	Compound	r_A	$V/(r_O + r_A)^3$	Compound	r_A	$V/(r_O + r_A)^3$
$AlSbO_4$	0.53	8.92	$ScAsO_4$	0.87	24.82	$ScVO_3$	0.87	25.43
$CrSbO_4$	0.615	8.27	$LuAsO_4$	0.97	23.80	$LuVO_4$	0.97	24.32
$GaSbO_4$	0.620	8.22	$YbAsO_4$	0.98	23.68	$YbVO_4$	0.98	24.19
$FeSbO_4$	0.645	7.98	$TmAsO_4$	0.99	23.62	$TmVO_4$	0.99	24.13
$RhSbO_4$	0.665	7.90	$ErAsO_4$	1.00	23.53	$ErVO_4$	1.00	24.08
			$YAsO_4$	1.015	23.27	YVO_4	1.015	23.83
			$DyAsO_4$	1.03	23.14	$DyVO_4$	1.03	23.60
			$TbAsO_4$	1.04	23.19	$TbVO_4$	1.04	23.58
			$GdAsO_4$	1.06	22.82	$GdVO_4$	1.06	23.30
			$EuAsO_4$	1.07	22.81	$EuVO_4$	1.07	23.24
			$SmAsO_4$	1.09	22.48	$SmVO_4$	1.09	22.95
σ_{n-1}	0.05	0.40	σ_{n-1}	0.06	0.63	σ_{n-1}	0.06	0.68
r*	−0.998		r	−0.996		r	−0.998	

Note: Structural data are from Wyckoff (1965). The ionic radii are Shannon and Prewitt's (1969) effective ionic radii.
* The term r is the linear correlation coefficient.

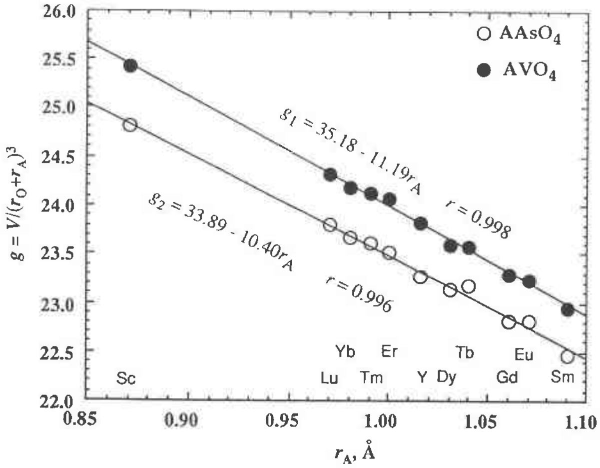

Fig. 2. Linear relationship between the ratio $V/(r_O + r_A)^3$ and r_A of compounds $AAsO_4$ and AVO_4 with tetragonal zircon structures. Structural data are from Wyckoff (1965).

$$f(r_A) = f(r_A^0) + (r_A - r_A^0)\frac{d}{dr_A}f(r_A^0) + \frac{1}{2!}(r_A - r_A^0)^2\frac{d^2}{dr_A^2}f(r_A^0) + \ldots$$

where r_A^0 is a specific value of r_A. Since $(r_A - r_A^0)$ is very small, the terms from the quadratic term on are negligible. We have:

$$f(r_A) \approx f(r_A^0) - r_A^0\frac{d}{dr_A}f(r_A^0) + r_A\frac{d}{dr_A}f(r_A^0)$$

$$= p + qr_A \qquad (p, q = \text{const.}).$$

The unit-cell volume is:

$$V = (p + qr_A)(r_X + r_A)^3 \qquad (p, q = \text{const.}) \tag{6}$$

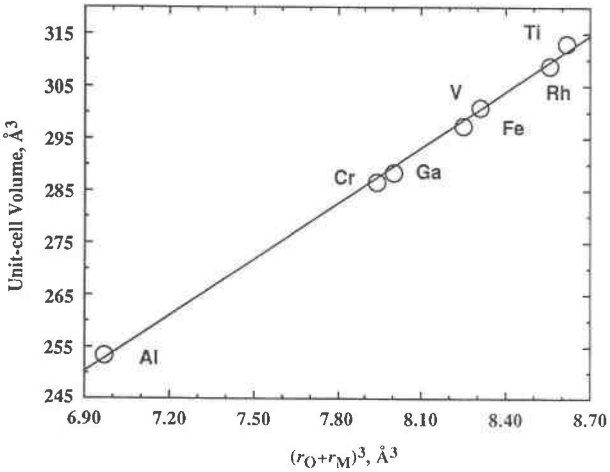

Fig. 3. Variation of the unit-cell volume with $(r_O + r_M)^3$ of oxides M_2O_3 with the corundum structure. Structural data are from Donnay and Donnay (1963).

TABLE 2. Ratio $V/(r_X + r_A)^3$ of binary compounds

NaCl structure		Corundum structure		Bixbyite structure	
Compound	$V/(r_X + r_A)^3$	Compound	$V/(r_X + r_A)^3$	Compound	$V/(r_X + r_A)^3$
NiO	7.87	Al_2O_3	36.37	Mn_2O_3	100.3
NbO	7.95	Cr_2O_3	36.12	In_2O_3	101.0
MgO	7.90	Ga_2O_3	36.08	Lu_2O_3	101.6
CoO	7.93	V_2O_3	36.08	Yb_2O_3	100.6
MnO	7.92	Fe_2O_3	36.27	Tm_2O_3	101.1
CdO	7.97	Rh_2O_3	36.13	Tl_2O_3	100.9
CaO	8.06	Ti_2O_3	36.35	Er_2O_3	100.9
EuO	8.02			Dy_2O_3	100.9
BaO	8.08			Tb_2O_3	100.6
				Eu_2O_3	101.4
				Sm_2O_3	101.0
$\bar{X}$	7.97	$\bar{X}$	36.20	$\bar{X}$	100.51
$\sigma_{n-1}/\bar{X}$	0.0091	$\sigma_{n-1}/\bar{X}$	0.0035	$\sigma_{n-1}/\bar{X}$	0.0082

Note: Structural data are from Donnay and Donnay (1963).

According to Equation 6, the ratio of $V/(r_X + r_A)^3$ will vary linearly with r_A, as is confirmed by actual crystal data. Listed in Table 1 are the $V/(r_O + r_A)^3$ ratios and the radii of A cations of compounds $ASbO_4$, $AAsO_4$, and AVO_4. The well-defined linearity is demonstrated by the linear correlation coefficients.

Figure 2 illustrates the variation of the $V/(r_O + r_A)^3$ ratio with r_A for compounds $AAsO_4$ and AVO_4 with the tetragonal zircon structure. The result is two reasonably well-defined straight lines with negative slopes. The slopes are always negative in the examples that have been considered. The explanation for the negative slopes may be that as the radius of cation A increases, the contribution to the volume of other cations is eclipsed because large ions can form a frame to accommodate other cations.

Based on Equation 6, it is easy to understand that the plot of V vs. $(r_X + r_A)^3$ should be a curve rather than a straight line, and that as q is negative, the curve is convex upward. The curvature is determined by the ratio p/q.

SIMPLIFICATION WITH BINARY COMPOUNDS

For binary isostructural compounds such as A_mX_p, Equations 1–3 reduce to:

$$a = \sum_i (r_X + r_A)\cos\alpha_i = (r_X + r_A)\sum_i \cos\alpha_i \tag{7}$$

$$b = \sum_i (r_X + r_A)\cos\beta_i = (r_X + r_A)\sum_i \cos\beta_i \tag{8}$$

$$c = \sum_i (r_X + r_A)\cos\gamma_i = (r_X + r_A)\sum_i \cos\gamma_i \tag{9}$$

According to the definition of Bloss (1971), isostructuralism or isotypism refers to two or more compounds having atoms arranged in the same type of crystal structure. In multi-cation compounds, different types of coordination polyhedra must link together so that the relative positions of atoms vary with the sizes of the cations. In binary compounds, on the other hand, the relative coordinates of atoms are almost identical in a given isostructural series. Along the same chain of bonds from (0,0,0) to (1,1,1), the angles defined by any bond, i.e., the

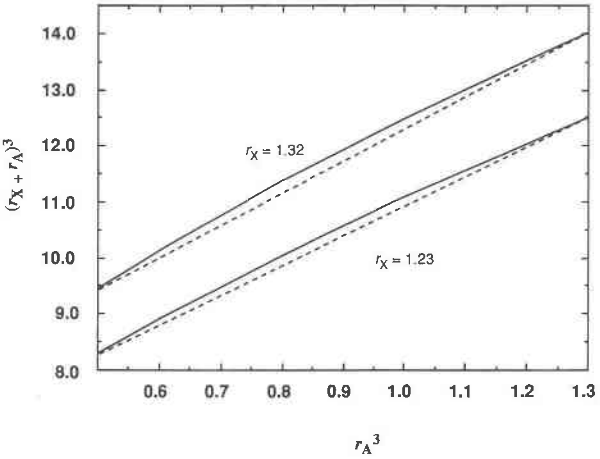

Fig. 4. Curves of $(r_X + r_A)^3$ vs. r_A^3. The two values of r_X are the radii of O^{2-} in sixfold coordination and of F^- in fourfold coordination, respectively. Both curves approximate a straight line.

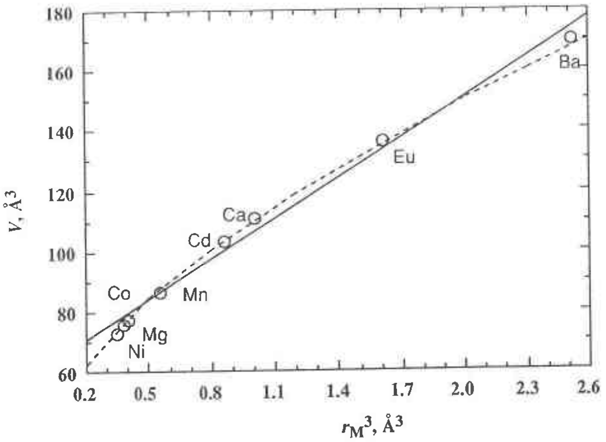

Fig. 5. Unit-cell volume vs. r_M^3 of oxides MO with the NaCl structure. Though the plot approximates a straight line, the theoretical relationship is given by the dashed curve. Structural data are from Donnay and Donnay (1963).

angles α_i, β_i, and γ_i in Equations 7–9, are approximately the same in different compounds. In addition, because of the approximation $\cos(\theta + \Delta\theta) \approx \cos\theta$ when $\Delta\theta$ is small, the cosine values remain approximately constant even if there are some variations of the angles. Then, based on Equations 7–9, the unit-cell volume formula for binary compounds becomes:

$$V = k(r_X + r_A)^3 \qquad (k = \text{const.}). \qquad (10)$$

For a series of isostructural compounds where the relative positions of all atoms are fixed, the validity of Equation 10 is self-evident. It is also valid when a structure has variable coordinates. Listed in Table 2 are data for three series of isostructural binary compounds with both fixed and variable structural parameters. The ratios of $V/(r_X + r_A)^3$ are approximately constant in a given series without obvious variation with the size of the cation. In Figure 3 unit-cell volumes are plotted against $(r_O + r_M)^3$ for oxides M_2O_3 with corundum structures. All points fall close to a straight line. In fact, Equation 10 is a simplification of Equation 6. The term qr_A in Equation 6 is a factor that reflects systematic variation of the structures. Since there is little variation in the case of binary compounds, this term approaches zero and Equation 10 results.

RELATIONSHIP BETWEEN V AND r_A^3

Shannon and Prewitt's (1969) linear relation between the unit-cell volume and r^3 is actually a first approximation. From Equation 10 it can be seen that a plot of V vs. r_A^3 will be virtually the same as a plot of $(r_A + r_X)^3$ vs. r_A^3 because V and $(r_A + r_X)^3$ are linearly related. When $(r_X + r_A)^3$ is plotted against r_A^3, the result is illustrated by the solid curves in Figure 4. The r_X values of the two curves are the radii of six-coordinated O^{2-} (1.40 Å) and four-coordinated F^- (1.31 Å), respectively. The actual relationship between $(r_X + r_A)^3$ and r_A^3 is a curve. The curvature is slight, however, and the curve approximates a straight line over a considerable range of ionic radii. The range of the abscissa of Figure 4 embraces the radii of many different cations. In addition, when experimental unit-cell volumes are plotted against r_A^3, the points usually will fluctuate about the true curve because of experimental errors. Thus the curvature is liable to be obscured and a linear relationship may be apparent. Figure 5 shows the variation of unit-cell volume with r_M^3 of oxides MO with NaCl structures. The straight regression line fits the data points relatively well. However, the actual relation is represented by the dashed curve whose equation is $V = 7.97(1.40 + r_M)^3$ with the coefficient 7.97 taken from Table 2.

For multiple compounds, as a result of the combination of the convex curves of V vs. $(r_X + r_A)^3$ and $(r_X + r_A)^3$ vs. r_A^3, the convex nature of the curve of V vs. r_A^3 is often rather obvious. Whether the deviation from linearity is displayed depends on the ratio p/q in Equation 6, the range of ionic radii, and the accuracy or consistency of the data.

APPROXIMATE LINEAR RELATIONSHIP BETWEEN V AND r_A

The equation involving unit-cell volume $V = k(r_X + r_A)^3$ for binary compounds contains a cubed term. A plot of such a function $y = ax^3$ is nearly a straight line beyond the point (1, a) if the range of x is not very large. Since the ionic radii of O^{2-} and F^- are all greater than 1, the curves of V vs. $(r_X + r_A)$ for oxides and fluorides all belong to the region exceeding the point (1, a). The relationship between V and r_A can then be replaced by a linear function; i.e.,

$$V = Ar_A + B \qquad (A,B = \text{const.}).$$

Figure 6 shows the variation of V with r_M of oxides MO_2 with the fluorite structure. The approach to linearity

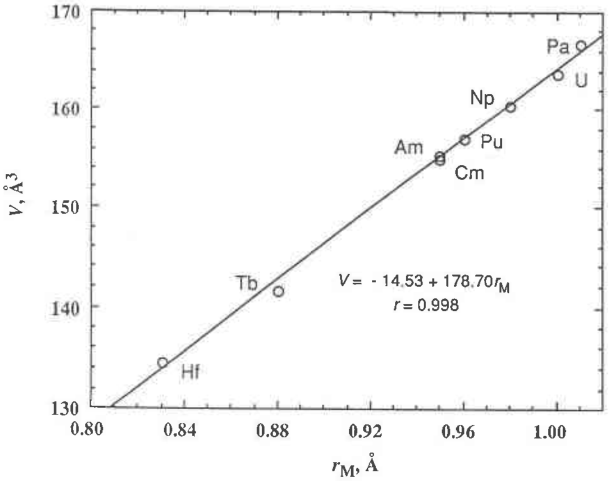

Fig. 6. Approximate linear relationship between the unit-cell volume and r_M of oxides MO_2 with the fluorite structure. Structural data are from Donnay and Donnay (1963).

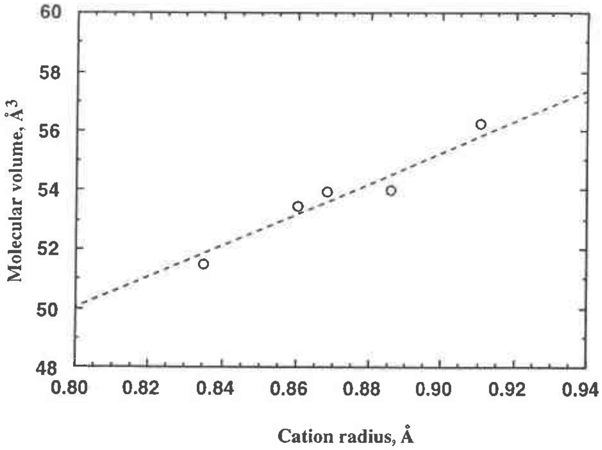

Fig. 7. Molecular volume vs. average cation radius of multi-cation calcite-type carbonates. The points fall close to the dashed regression line of single-cation calcite-type carbonates. Structural data are from JCPDS (1950–1986) and Winchell and Winchell (1964).

is very good. The regression equation is $V = 178.70r_M - 14.52$, with a linear correlation coefficient of $r = 0.998$.

For multiple compounds, the curvature of V vs. $(r_X + r_A)^3$ is slight. In addition, the convex nature of the plot for this curve and the concave curvature of the curve for the cubed function partially offset each other. The relationship between V and r_A therefore also approximate a linear function, as demonstrated by the following examples for carbonates.

ADDITIVITY OF THE MOLECULAR VOLUMES OF CARBONATES

The relationship between the molecular volume and cation radius is linear for carbonates with the calcite structure (Table 3). An interesting result is that carbonates with more than one type of cation fall on the line defined by mono-cation carbonates within an isotypic series. In Figure 7 the molecular volumes of carbonates with the calcite structure and having more than one kind of cation are plotted vs. the average cation radius. The data points are on the line obtained by linear regression of the data for carbonates with a single cation species. This suggests that the average effect of two or more cations is equal to that of a cation with an average radius. It is easy to prove that this is sufficient and necessary for condition that the separate molecular volumes of single-cation carbonates can be added to give the volume of the multi-cation carbonate.

TABLE 3. Linear relationship between the molecular volume and cation radius for carbonates with the calcite structure

	Cation radius (Å)	Molecular volume (Å³)
$NiCO_3$	0.700	44.92
$MgCO_3$	0.720	46.51
$CoCO_3$	0.735	46.84
$ZnCO_3$	0.745	46.95
$FeCO_3$	0.77	47.22
$MnCO_3$	0.82	51.59
$CdCO_3$	0.95	56.95
$CaCO_3$	1.00	61.31
Linear correlation coefficient		0.991

Note: Structural data are from JCPDS (1950–1986).

If the coordinations of cations in the component single-cation carbonates are the same as in the multi-cation carbonates, the additivity relation gives values close to observed ones. In Table 4 the molecular volumes obtained through addition are compared with experimental values and they can be seen to be very similar.

The coordination of a cation should be the same for the component carbonates and multi-cation carbonates if the resultant multi-cation molecular volumes are to be accurate. However, when a carbonate occurs as polymorphs, their molecular volumes do not differ very much. For example, the molecular volumes of calcite and vaterite, 61.31 and 62.63 Å³, respectively, are similar. A general additivity relation is therefore possible. Regardless of the coordinations of cations, the molecular volume of a multi-cation carbonate can be obtained by summing the molecular volumes of the component single-cation carbonates.

TABLE 4. Comparison of the calculated and observed molecular volumes (Å³) of multi-cation carbonates

	V_{calc}	V_{obs}		V_{calc}	V_{obs}
$CaMg(CO_3)_2$	107.6	107.0	$CaBa(CO_3)_2$	132.8	133.7
$Ca(Mg_{0.67}Fe_{0.33})(CO_3)_2$	108.4	107.9	$PbMg(CO_3)_3$	113.9	115.9
$CaFe(CO_3)_2$	109.8	107.4	$BaMg(CO_3)_2$	122.6	121.9
$CdMg(CO_3)_2$	103.6	103.0	$BaMn(CO_3)_2$	127.7	132.4
$CaMn(CO_3)_2$	112.7	112.5	$MgSr(CO_3)_2$	111.3	114.2

Note: Structural data are from JCPDS (1950–1986) and Winchell and Winchell (1964).

TABLE 5. Comparison of the calculated and experimental molecular volumes (Å³) of complex carbonates

Formula	$V_{calc.}$	$V_{obs.}$	Relative difference (%)	Formula	$V_{calc.}$	$V_{obs.}$	Relative difference (%)
$Ca(Mn_{0.88}Mg_{0.12})(CO_3)_2$	111.7	111.0	+0.63	$Ca_2Cu(UO_2)(CO_3)_4 \cdot 6H_2O$	400.8	412.9	−2.93
$Na_2Ca(CO_3)_2 \cdot 5H_2O$	249.7	246.8	+1.18	$CaUO_2(CO_3)_2 \cdot 3H_2O$	219.2	219.9	−0.32
$Na_2Cu(CO_3)_2 \cdot 3H_2O$	197.9	204.3	−3.13	$K_2Ca_3(UO_2)_2(CO_3)_6 \cdot 9H_2O$	697.8	696.8	+0.14
$Na_2Mg(CO_3)_2$	113.1	115.7	−2.25	$Ca_2Ce_3(CO_3)_5F_3$	337.7	339.5	−0.53
$Na_2Ca_2Sr_2(CO_3)_5$	309.6	306.9	+0.88	$K_2Mg(CO_3)_2 \cdot 4H_2O$	243.7	240.9	+1.16
$K_2Ca(CO_3)_2$	151.0	151.4	−0.26	$KNaCO_3 \cdot 6H_2O$	234.4	235.4	−0.42
$Mg_3Ca(CO_3)_4$	200.7	204.0	−1.47	$K_3NaUO_2(CO_3)_3 \cdot H_2O$	294.9	309.4	−4.69
$CaBi_2O_2(CO_3)_2$	159.3	155.8	+2.25	$Na_2Cu(CO_3)_2 \cdot 3H_2O$	189.5	204.3	−7.24
$Li_2Cr(CO_3)_2 \cdot 3H_2O$	200.1	194.2	+3.04	$NaCaSr_3Y(CO_3)_6 \cdot 3H_2O$	446.6	427.2	+4.54
$KAgCO_3$	84.8	86.5	−1.97	$LiKCO_3$	76.4	77.4	−1.29
$Ca_7Ba_6(CO_3)_{13}$	853.3	836.3	+2.03	$MgSr(CO_3)_2$	111.3	114.2	−2.54
$BaCe(CO_3)_2F$	147.8	147.2	+0.41	$K_2Mg(CO_3)_2$	140.8	132.7	+6.10
$Ca_2Ce_3(CO_3)_5F_3$	337.7	339.5	−0.53	$K_2Sr(CO_3)_2$	159.1	167.4	−4.96
$CaYF(CO_3)_2$	120.4	124.6	−3.37	$RbAgCO_3$	91.7	93.5	−1.93
$CaZn(CO_3)_2$	108.3	107.4	+0.84	$NaAgCO_3$	72.2	74.5	−3.09

Note: Data are from JCPDS (1950–1986) and Winchell and Winchell (1964).

Listed in Table 5 are the calculated and experimental molecular volumes of 30 multi-cation carbonates. The molecular volume of H_2O in hydrates is taken as 24.40 Å³ (Zhang and Ye, 1985). The additivity relation still holds, although the precision of the relation is diminished.

SUMMARY

The relationship between the unit-cell volume and the radius of cation A of a multi-cation isostructural series is $V = (p + qr_A)(r_X + r_A)^3$, where p and q are constants. The equation for binary isostructural compounds is $V = k(r_X + r_A)^3$, where k is constant. Because the curve of $(r_X + r_A)^3$ vs. r_A^3 is nearly a straight line, the unit-cell volume is empirically linearly correlated with r_A^3. A nonlinear relation for multiple compounds is usually observed. The curve of V vs. r_A is the curve for a cubed function and is nearly a straight line in all cases where the present discussion is applicable. It is safe to say that V is approximately linearly correlated with r_A. Multi-cation carbonates plot on the line of molecular volume vs. r_A formed by mono-cation carbonates with the same structure. This implies that the molecular volumes of multi-cation carbonates are additive. If the coordinations of the cations in the component carbonates are the same as in the multi-cation carbonates, the additivity relation is quite accurate. A general additivity relation, i.e., one independent of the coordination, is also acceptable, though with slightly lower precision.

REFERENCES CITED

Bloss, F.D. (1971) Crystallography and crystal chemistry. Holt, Rinehart and Winston, Inc., New York.

Donnay, J.D.H., and Donnay, G. (1963) Crystal data: Determinative tables, (2nd edition). American Crystallographic Association, Washington, DC.

Hazen, R.M., and Finger, L.W. (1982) Comparative crystal chemistry. Wiley, New York.

JCPDS. (1950–1986) Powder diffraction file, sets 1–36, Inorganic volume. International Center for Diffraction Data, Philadelphia.

Prewitt, C.T. (1985) Crystal chemistry: Past, present, and future. American Mineralogist, 70, 443–454.

Shannon, R.D., and Prewitt, C.T. (1969) Effective ionic radii in oxides and fluorides. Acta Crystallographica, B25, 925–946.

Winchell, A.N., and Winchell, H. (1964) The microscopical characters of artificial inorganic solid substances. Academic Press, New York.

Wyckoff, R.G. (1965) Crystal structures, vol. 3 (2nd edition). Interscience Publishers, New York.

Zhang, Z.Y., and Ye, D.N. (1985) An investigation of the additivity of the molecular volumes of sulfates. Scientia Geologica Sinica, 2, 180–189.

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