The Concept of a "Derivative Structure"

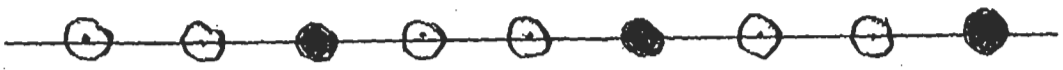
Certain more complex structures can be related to simpler, more symmetric structure by a perturbation of one sort or another. We intuitively recognize this in statements such as "the rock salt structure of NaCl looks just like a primitive cubic array of spheres except every other black sphere is replaced by a red one." NaCl may thus be said to be "derived" from a simple cubic array of atoms.

The concept is useful in extending our understanding of simple structures to ones that are progressively more complicated. It is mainly useful, however, because it provides a powerful approach to the determination of certain kinds of structures from diffraction data

There are four types of perturbations that may be employed separately or in concert to form a derivative. These may be illustrated with one-dimensional structures

Basic Structure

Substitution Derivative



Omission Derivative

ADDITION DERIVATIVE ("STUFFING")

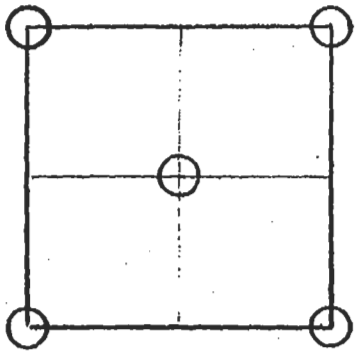
DISTORTION DERIVATIVE

Although it might seem that ANY structure may be regarded as a Derivative of Any other, the term (introduced by M.J. Buerger) is reserved for cases in which the perturbation results in suppression of SYMMETRY operations that existed in the basic or fundamental structure have been removed. The derivative structures may be seen to have lost some of the loci in the basic structure across which the entire structure could be reflected left-to-right and remain invariant. Also, the translational periodicity of the derivatives has increased. Structures for which this is true are called SUPERSTRUCTURES. Derivative structure thus, by definition, have a lower density of SYMMETRY operations than the parent structure.

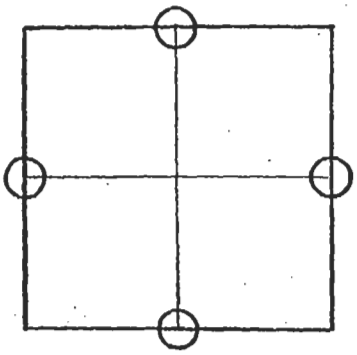
Twelve figures of crystal structures removed for copyright reasons.

Please see: Wuensch, B. J. "The crystal chemistry of Sulfur." Chapter 16A in *Handbook of Geochemistry*. Vol. II/3. Berlin, Germany: Springer Verlag, 1972.

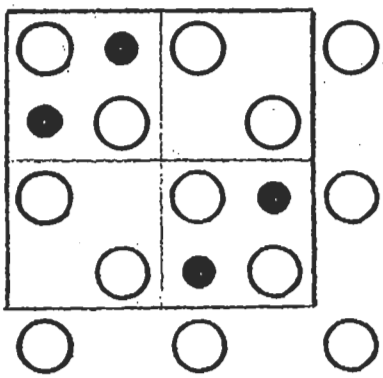
○ Mg^{2+} ● Al^{3+} ○ O^{2-}



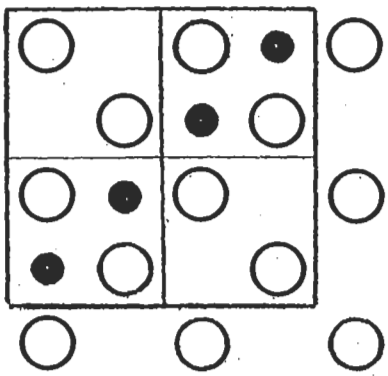
$z = 0$



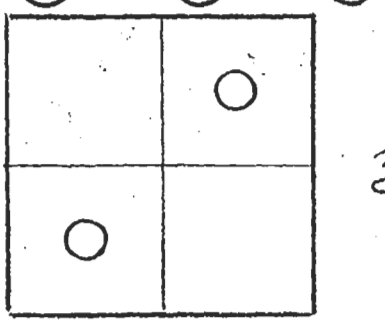
$z = \frac{4}{8}$



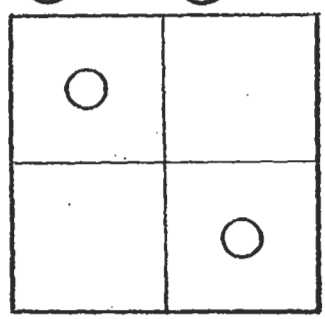
$z = \frac{1}{8}$



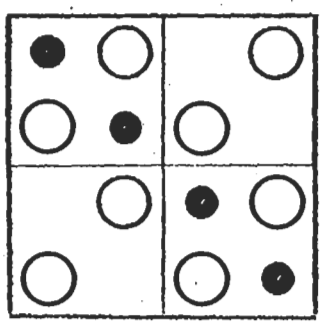
$z = \frac{5}{8}$



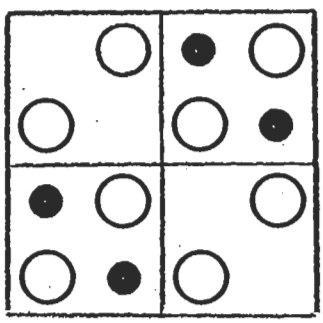
$z = \frac{2}{8}$



$z = \frac{6}{8}$



$z = \frac{3}{8}$



$z = \frac{7}{8}$

SPINEL $MgAl_2O_4$

$a = 8.083$ Å

$Fd\bar{3}m - O_h^7$

Mg^{2+} IN 8a $\bar{4}3m$ 000

Al^{3+} IN 16d $\bar{3}m$ $\frac{1}{8}\frac{1}{8}\frac{1}{8}$

O^{2-} IN 32e 3m xxx $x \approx \frac{3}{8}$