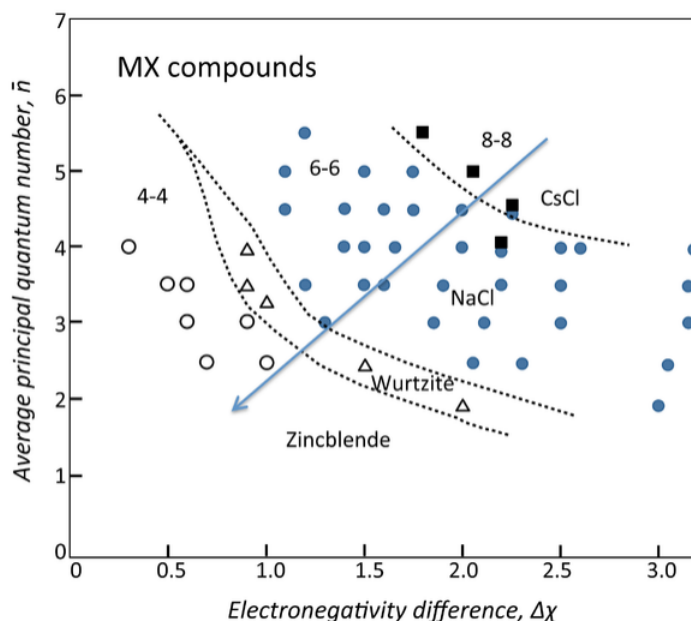


9.2: Structure Maps

Structure maps, which plot structures against properties such as electronegativity, are more consistent than radius ratio rules in correctly predicting coordination numbers and crystal structures. One of the early examples of this approach was published by Mooser and Pearson in 1959.^[3]

A **Mooser-Pearson diagram** maps crystal structures according to the average principal quantum numbers of the atoms and their electronegativity difference. The basic ideas behind such a plot are:

- The greater the electronegativity difference, the more ionic is the compound. Higher ionicity results in higher coordination numbers because anions like to surround cations (and vice versa).
- Higher principal quantum numbers result in less s-p hybridization, less directional bonding, and therefore higher coordination number. We saw this trend before with the structures of elements in group IV: descending the group the coordination number increases progressively from 3-4 (carbon) to 12 (Pb).



The lines in the Mooser-Pearson diagram separate MX compounds with CsCl, NaCl, and tetrahedral (wurtzite and zincblende) structures. Note that wurtzite has higher ionicity than zincblende in the plot, consistent with our discussion of the "boat" and "chair" ring structures in Chapter 8. Diamorphic compounds tend to fall on the boundaries. On the whole, the Mooser-Pearson diagram makes far fewer errors in predicting structures than the radius ratio rule. There are similar diagrams for MX_2 structures, in which the order of ionicity is CaF_2 (8:4 coordination) > rutile (6:3) > silica structures (4:2).

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