

Density of minerals VIII: The significance of crystal structure

In the first page of this series, we saw that density of simple carbonate minerals is roughly proportional to atomic weight of the inter-radical cation (for example, Pb^{2+} in cerussite). On this page, the emphasis is on the "roughly" in "roughly proportional". For example, one might look at the upper plot here and ask "Why are magnesite and aragonite denser than one would expect from the regression lines for the rhombohedral and orthorhombic groups, respectively?" or "Why are calcite, otavite, and witherite less dense than expected?".

The answer to these questions can be seen in the lower plot, where the anomaly or residual in the upper diagram is plotted against cation radius. Among the rhombohedral carbonates, where the inter-radical cation is in six-fold coordination, smaller cations like Mg^{2+} let the structure collapse to give a proportionately large density. On the other hand, larger cations like Cd^{2+} and Ca^{2+} stretch the rhombohedral structure to give a proportionately small density. The same happens among the orthorhombic carbonates, where the inter-radical cation is in nine-fold coordination. In that case, Ca^{2+} is a relatively small cation and allows collapse of the structure and an anomalously great density, whereas a relatively large cation like Ba^{2+} stretches the structure to give a proportionately small density. Thus the details or anomalies of the trends in density in the upper plot are explained by the relationship of cation size to mineral structure shown in the lower plot.

