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Revision of Y^{3+} ionic radii in common minerals based on trace element partitioning

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ABSTRACT

The ionic radii of rare earth elements (REE: Sc, Y, and the lanthanides) are key to interpreting partitioning behavior between minerals and melts for use as petrogenetic tracers and thermometry. Of REE, Y commonly has the highest concentration and serves as a reference against which other REE concentrations or partition coefficients can be compared. Here, we show that published experimental data on mineral-melt partitioning of REE imply the ionic radius of Y^{3+} is smaller than commonly assumed by 0.001 Å for sixfold coordination to 0.005 Å for eightfold and ninefold coordination. This difference reconciles the partitioning behavior of Y^{3+} with that of other REE and improves reference states for interpreting trace element systematics in rocks. Thermobarometry can be highly sensitive to assumed ionic radii, and downward correction of the Y^{3+} ionic radius improves some REE-based temperatures by hundreds of degrees. Future studies that employ the most common tabulations of ionic radii of the REE (Shannon 1976) should use an ionic radius of Y^{3+} of 0.899, 1.014, and 1.070 Å for six-, eight-, and ninefold coordination, respectively; alternatively, the ionic radius of Y can be scaled to that of $Ho^{3+} \times 0.9984$. More generally, trace element partitioning data, coupled with theoretical models, provide an exact method for refining effective relative ionic radii in minerals where direct structural determinations are not possible.

Keywords: Yttrium, rare-earth element, mineralogy, ionic radius, geothermometry