Impact of Extreme Pressure on Bonded Radii of Atoms

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In order to understand the geochemistry of oxides at the extreme pressures encountered in the Earth's interior, a knowledge of how bonded radii of atoms respond to pressure is needed. Herein, we present results from theoretical calculations of how the bonded radii of Si and O in the SiO_2 polymorphs respond to pressures up to 100 GPa. The Si and O atoms are found to be highly rigid and incompressible. In stishovite, for example, Si and O decrease by 0.05 Å and 0.08 Å, respectively, between 0 and 100 GPa. The impact of extreme pressure on the bonded radii of Al, Ca, La, Sn, and Y atoms in a series of aluminate perovskites has also been examined at high pressure. Each study verifies how little the bonded radii change with pressure. In $YAlO_3$ perovskite, for example, the Y and Al bonded radii decrease by 0.05 Å and 0.11 Å, respectively, between 0 and 80 GPa. The calculations also indicate a change in coordination of Y with O from 9 to 10 at 20 GPa. The impact of these results on our understanding of the crystal chemistry of oxides under extreme pressure conditions will be discussed.