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Effective pair potential for Ca-O bonds in $CaGeO_3$ perovskite, garnet, wollastonite

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The $CaGeO_3$ perovskite and garnet were synthesized in a cubic anvil type apparatus under high pressure. The measurements of Ca and Ge K- edge XAFS spectra were carried out in the transmission mode at temperature up to 700 K. The effective pair potentials V(u)=au^2/2+bu^3/3!, for Ca-O bond in various phases of $CaGeO_3$ have been investigated by the temperature dependence of EXAFS Debye-Waller factors. The potential coefficient a for the Ca-O bond in perovskite-type $CaGeO_3$ is small, 4.4 eV/A^2, compared with those in garnet (6.0 eV/A^2) and wollastonite (6.4 eV/A^2). The potential for Ca-O bond in perovskite is broader than those in other $CaGeO_3$ polymorphs, which is one reason for the Clausius-Clapeyron's curve for perovskite-garnet phase boundary having a negative slope. The potential coefficients for the Ca-O in perovskite are significantly smaller than those for the longer Ge-Ge distances as the framework vibration though the potential coefficient decreases usually as a result of the larger bond distance.