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"Cs-tetra-ferri-annite:" High-pressure and high-temperature behavior of a potential nuclear waste disposal phase

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Abstract

Structure deformations induced by pressure and temperature in synthetic ''Cs-tetra-ferri-annite'' 1M $[Cs_{1.78}(Fe^{2+}_{5.93}Fe^{3+}_{0.07})(Si_{6.15}\ Fe^{3+}_{1.80}Al_{0.05})O_{20}(OH)_4]$, space group *C*2/*m*, were analyzed to investigate the capability of the mica structure to store the radiogenic isotopes ^{135}Cs and ^{137}Cs. ''Cs-tetra-ferri-annite'' is not a mineral name, but for the sake of brevity is used here to designate a synthetic analog of the mineral tetra-ferri-annite. The bulk modulus and its pressure derivative determined by fitting the unit-cell volumes between 0 and 47 kbar to a third-order Birch-Murnaghan equation of state are $K_0 = 257(8)$ kbar and $K_0' = 21(1)$, respectively. Between 23 °C and 582 °C, the *a* and *b* lattice parameters remain essentially unchanged, but the thermal expansion coefficient of the **c** axis is $\alpha_c = 3.12(9) \times 10^{-5}$ °C^{-1}. High pressure (*P*) and high temperature (*T*) produce limited internal strain in the structure. The tetrahedral rotation angle, α, is very small and does not change significantly throughout the *P* and *T* range investigated. Above 450 °C in air, ''Cs-tetra-ferri-annite'' underwent an oxidation of octahedral iron in the M2*cis* site, balanced by the loss of H and shown by a decrease of the unit-cell volume.

Independent isobaric data on thermal expansion and isothermal compressibility data define the ''geometric'' equation of state for ''Cs-tetra-ferri-annite'': $V/V_0 = 1 + 3.0(1)\ 10^{-5}\ T - 2.68(9)\ 10^{-3}\ P + 2.0(2) \times 10^{-5}\ P^2$ where *T* is in degrees Celsius, *P* is in kilobars. The α/β ratio of about 12 bar/°C indicate that the cell volume of ''Cs-tetra-ferri-annite'' remains unchanged under geothermal gradients of ~23 °C/km. On the whole, the data confirm that the structure of ''Cs-tetra-ferri-annite'' may be a suitable candidate for the storage of large ions, such as Cs in the interlayer and should be considered as a potential Synroc component.