

Problem Set 10

Ch 153a – Winter 2023

Due: 10 March, 2023

1. The Ti(III) oxidation state is rare in terrestrial minerals due to the comparatively highly oxidizing environment on Earth. Trivalent titanium does occur in extraterrestrial materials; one example is a titanium pyroxene found in the Allende meteorite. The empirical formula for this mineral is $\text{Ca}_{1.01}\text{Mg}_{0.38}(\text{Ti}^{3+})_{0.34}(\text{Ti}^{4+})_{0.14}\text{Al}_{0.87}\text{Si}_{1.26}\text{O}_6$. The crystal structure reveals that this mineral contains chains of edge-shared distorted octahedra with $\text{Ti}^{3+/4+}$ ions at the center. The Ti-Ti distance is 3.15 Å. The polarized single-crystal absorption spectra of the Ti^{3+} - Ti^{4+} pyroxene from the Allende meteorite at different pressures are shown below (α and β refer to two different polarization directions).

Propose assignments for the absorption bands at 14,000, 16,000, and 20,000 cm^{-1} (1 bar). On the basis of your assignments, offer explanations for the pressure dependent behavior of the three bands.

