Extraterrestrial and Terrestrial Fassaite Compared: Allende CV3 versus Fassa Valley, Italy.

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Introduction: Meteoritic Al-, Ti-rich clinopyroxene, first reported in CAIs in the Allende and VigaranCV3 chondrites, was termed “fassaite” and found to be structurally similar to terrestrial fassaite by crystal structure refinement [1]. Unlike terrestrial fassaite, it lacks Fe but contains significant Ti2+ and Ti4+ [1,2]. Al enters both the octahedral and tetrahedral sites via Tschermak’s substitution, along the diopside (Di: CaMgSi2O6) - Ca-Tschermak (CaTs: CaAlSi2O6) join. We report the crystal structure of fassaite from Allende inclusion TS62B and from the type locality, the Fassa Valley in Italy, by single crystal X-ray diffraction (XRD), as well as cation ordering by 29Si and 27Al Magic Angle Spinning (MAS) Nuclear Magnetic Resonance (NMR) and triple quantum (3Q) MAS NMR spectroscopy.

Methods: 29Si and 27Al MAS NMR spectra were collected on Allende fassaite using a 21.1 T (H at 900 MHz) Bruker Avance II NMR Spectrometer at the Canadian National Ultrahigh-Field NMR Facility for Solids. ~4 mg of sample (TS62B), scraped from the surface of a “potted butt”, was packed in a 2.5 mm MAS rotor. Other NMR conditions were chosen to ensure quantitative spectra. 29Si and 27Al MAS NMR spectra for terrestrial fassaite were collected on the Infinity Plus 400 (H at 400 MHz) and Inova 600 (H at 600 MHz), resp. at The University of Western Ontario.

Approx. 100 μm crystals of Allende and Fassa valley fassaite, showing no twinning, were chosen for single crystal XRD using a Bruker Kappa Apex II diffractometer with MoKα radiation.

Results and Discussion: The 29Si MAS NMR spectrum of Allende fassaite exhibits three peaks (FWHM ~ 3 ppm), representing three distinct Si environments, whereas Fassa Valley fassaite exhibits only a broad single peak (FWHM ~ 10 ppm) where distinct Si environments are unresolved. 27Al MAS and 3QMAS NMR spectra of Allende fassaite show two distinct sets of well resolved peaks representing octahedral and tetrahedral environments. The 27Al MAS NMR of Fassa Valley fassaite is less well resolved. Refinements of single crystal XRD data, however, indicate that both fassaite samples have the same symmetry, C2/c, and comparable unit cell dimensions (~ a 9.8 Å, b 8.8 Å, c 5.3 Å).

Both Allende and Fassa Valley fassaite appear to be long-range disordered as evidenced by C2/c symmetry [3]. The well-resolved narrow NMR peaks from Allende fassaite indicate local ordering of Si and Al cations on the tetrahedral chain. Fassa Valley fassaite appears disordered, implying that Si and Al are randomly distributed, resulting in peak broadening, consistent with other results [4]. Additional NMR peak broadening in terrestrial fassaite might be due to a higher Fe content (Feopt < 5 wt%). This is reflective of the different evolution conditions for Allende vs Earth.

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