CALCULATING MINERALOGY OF EXO-CAIs USING THERMOSNCC. G. Boyer[1], C. Unterborn[1], and S. Desch[1] [1] School of Earth and Space Exploration, Arizona State University, Tempe AZ 85287. gmboyer@asu.edu

Introduction: The first solids formed in the solar system are calcium-rich, aluminum-rich inclusions, or CAIs, found in most chondrites. These inclusions formed from aggregations of condensates bearing minerals, such as corundum [Al_2O_3], hibonite [$CaAl_{12}O_{19}$], grossite [$CaAl_4O_7$], perovskite [$CaTiO_3$], or calcium monoaluminate ("CA1") [$CaAl_2O_4$] [1]. These minerals are rich in refractory elements such as Ca, Al, Ti, and rare earth elements that are predicted to condense at high temperatures well above 1400 K, as depicted in Figure 1 [1].

Refractory elements were fractionated to a high degree within the solar nebula: the mass ratios Ca/Mg, Al/Mg, Ti/Mg, etc., are uniformly depleted in enstatite chondrites by as much as 24%, and uniformly enriched in carbonaceous chondrites, by up to 38% in CV chondrites, relative to the same ratios in CI chondrites [2]. These variations among chondrites, up to 60%, represent some of the largest fractionations seen among major rock-forming elements in primitive planetary materials. The variations have been attributed by [3] to radial displacement within the Sun's protoplanetary disk of CAIs themselves, as refractory minerals can comprise a large fraction (8 wt%) of the mass of solids, and these refractory-rich solids are the first to grow to sizes that allow them to aerodynamically decouple from the gas.

This implies that the largest variations in the compositions of planetary materials in exoplanetary systems may also be due to radial movement of objects — "exo-CAIs"— formed from the first minerals to condense in those systems' protoplanetary disks. Different stars, however, have different chemical abundances; molar ratios (e.g., Mg/Si) can vary by a factor of two from the ratios in the Sun [4]. Even within the solar nebula there was a range of redox states due to movement of water [5]. Thus, it is possible that exo-CAIs make up a different fraction of the mass of solids and could have different mineralogies. To assess the magnitude of refractory element fractionations and compute the degree of fractionations of specific elements, we will use the new code we are developing, ThermoSNCC, to compute the condensation sequence of refractory minerals for different observed stellar compositions.

Introducing ThermoSNCC: There currently is no free, open-source, easily accessible software available for modeling multi-phase equilibrium for typical cosmochemical conditions. This makes it difficult to test ideas about how condensation might be affected by pressure and oxidation state in the early solar system, and across the wide range of chemical compositions of different exosystems.

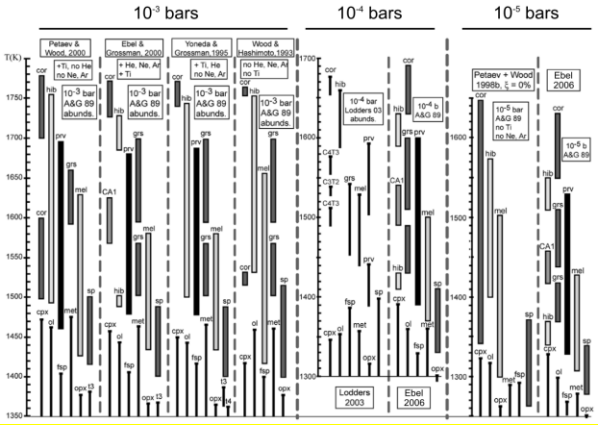

Figure 1. Comparison of condensation sequences of refractory minerals calculated in the literature from stellar gas of solar composition. Adapted from [1].

Here we apply the Thermodynamic Solar Nebula Condensation Calculator (ThermoSNCC), a free, open-source software tool we are developing for modeling solid-liquid-gas equilibrium under low pressure (<1 bar), high temperature (>1000 K) conditions [6]. It introduces a self-consistent ideal gas solution into the full suite of solid and liquid phases of the MELTS thermodynamic equilibration framework [7] available through the online ENabling Knowledge Integration (ENKI) JupyterHub environment. This ensures users will be able to perform calculations entirely through an internet browser, as shown in Figure 2. Model customization and multi-phase equilibrium calculations in ThermoSNCC are both handled via open-source software tools in the form of Jupyter Notebooks that can be copied, modified, and shared among collaborators. Calculating a condensation sequence is as simple as selecting an initial gas composition, pressure, and temperature range, and then executing a digital notebook. Coding knowledge is not required. Additionally, elemental abundances of stars listed in the Hypatia Catalog [4, 8, 9] can be imported directly as compositional input, as was done in this study.

Results: Equilibrium condensation calculations for exo-CAIs were performed for a system containing H, He, O, Ne, Mg, Al, Si, Ar, Ca, and Ti. We found that this set was complete enough to produce sequences resembling published benchmark calculations for re-

fractory element condensation [1] while minimizing time spent re-compiling model code after tweaks and optimizations.

Condensation sequences were calculated from elemental compositions of 150 random stars sampled from the Hypatia catalog. All sequences began at a 2000 K and decreased in 5 K intervals while maintaining a total pressure of 10^{-5} bars. Our preliminary calculations suggest that exo-CAI condensation sequences are largely similar across the vast majority of stars in the Hypatia catalog. Ratios of Al, Ca, Si, Ti, and O to Mg were consistent enough that there was little variation in the condensation order of minerals typical of CAIs. Starting with the solar composition reported for our sun [10], our model predicts the appearance of corundum first, followed by hibonite, and then perovskite plus grossite with decreasing temperature. This general condensation sequence was also observed across our randomly-sampled set of star compositions. This is encouraging, as it could indicate many of our assumptions about CAI fractionation in our solar system apply to the vast majority of exosystems.

While the sequences themselves did not vary much, condensation temperatures fluctuated based on differences in the partial pressures of CAI-forming elements in the gas mixture. We observed that increasing O/H ratios resulted in elevated condensation temperature. For instance, the two stars with the greatest difference in the molar abundance of oxygen in our sample set, HIP 80818 (O/H $= 10^{8.73}/10^{12}$) and HIP 60591 (O/H = $10^{9.14}/10^{12}$), also had the largest temperature shift (+150 K) in the initial appearance of corundum.

In addition to random sampling, we extended our calculations to several hand-picked stars where we noted extreme ratios of CAI-forming elements relative to our sun. Our goal was to qualitatively assess unusual characteristics in the condensation sequences of these outlier stars that would set them apart from the random samples. For example, HIP 111282 is a star with a low Ca/Al ratio that produced a condensation sequence with a diminished stability region of Ca-bearing minerals like hibonite, grossite, and perovskite in favor of corundum. Similarly, the elevated ratio of Ti/Ca of HIP 20349 enhanced the thermodynamic stability of Ti-bearing perovskite in the perovskite + grossite temperature region.

As we continue to make improvements to ThermoSNCC and explore condensation sequences of both mundane and unusual star compositions, predictable patterns may begin to emerge that will inform theories about CAI-formation, fractionation, and available materials for planet formation in exosystems and our early solar system.

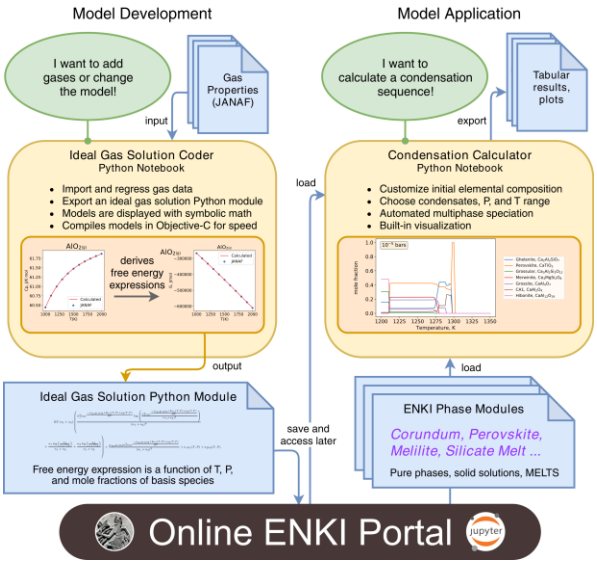

Figure 2. Example workflow for model development and application with ThermoSNCC using the online ENKI platform.

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