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Experimental determination of crystal structure and thermodynamic properties of carbonaceous chondrite parent body, wadalite

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The mineral wadalite ($Ca_6Al_5Si_2O_{16}Cl_3$) was first discovered in a skarn xenolith[1], but has excited interest due to its presence in a carbonaceous chondrite asteroid meteorite, where it evidences reactions with Cl-rich fluids[2]. Wadalite can also act as a weakly-hydraulic Cl-carrier in calcium-sulfo-aluminate-based cements[3]. Wadalite forms a solid solution with Cl-mayenite ($Ca_{12}Al_{14}O_{32}Cl_2$), in which tetrahedral Si^{4+} is replaced by Al^{3+} and a vacancy cage replaces Cl^-. Determining the crystal structure and thermodynamic properties of wadalite and its solid solution is crucial to volcanology, planetary science and cement communities. To investigate the thermodynamic properties, we synthesised pure wadalite and Cl-mayenite by the acid-catalysed sol-gel method at 820 °C, with a 5-6 hour dwell time. We then measured thermodynamic properties (e.g., heat capacity, entropy, and enthalpy) of wadalite using a Quantum Design physical property measurements system (PPMS) at ISIS, Diamond Light Source, Oxford, from 0 to 300 K, and a Netzsch Differential Scanning Calorimeter from 300K to 1873 K at the University of Texas at San Antonio. Thermodynamic data were then combined with the enthalpy of formation results from Density Functional Theory (DFT) and previous experiments to model the thermodynamic properties of wadalite using the 3rd generation CALPHAD function.

Our Rietveld quantification phase analysis shows that the synthesised wadalite and Cl-mayenite are ~98% pure with grain sizes of ~78 nm. The pure phase required some atomic occupancy refinement to fit the diffractogram, which impacts the centrosymmetric nature of wadalite crystals. The BSE (back-scatter) image of powder wadalite grains showed small grains growing on the tops of large grains due to Ostwald Ripening. The heat capacity of wadalite shows an onset of melting at 1150 °C, followed by phase transformations to mayenite, alinite, and Cl-mayenite from 1200 to 1550 °C, with complete melting at ~1600 °C. This study sheds light on the stability and potential behaviour of wadalite and its solid solutions, providing new thermodynamic information needed to model processes on planetary surfaces and in the cement industry.

References:[1] Tsukimura et al. (1993) Acta Crystallographica, C49, 205-207; [2] Ishii et al. (2010) American Mineralogist; [3] Simoni et al. (2021) CCR;