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MELTS+DEW: Modeling major element+Cl+F+S phase equilibria, redox reactions and elemental partitioning in magmatic-hydrothermal systems

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The silicate liquid thermodynamic model in the MELTS model collection [1] is combined with the Deep Earth Water (DEW) model [2] and extended to estimate elemental partitioning of Cl, F, and S between melt, aqueous fluid and mineral phases. This model is applicable to the compositions of natural magmas. It includes provision for S in multiple oxidation states, and quantifies the coupling of sulfide and sulfate to ferrous and ferric iron in the melt. The fugitive components are treated as trace constituents in the melt phase, which affords considerable simplification in model structure and significantly reduces the number of required model parameters. Standard state properties of novel components and species are calibrated from fluid-melt partitioning experiments, mineral phase equilibria, and experimental studies of melt coexisting with sulfide liquid (SL). Data from the last set of studies render the thermodynamic model internally consistent with the SL model of Kress and others [3]. The partitioning of electrons amongst sulfide, sulfate, ferrous and ferric melt species is achieved via the condition of homogeneous equilibrium. Because chemical potentials of all melt components must be equivalent in all coexisting phases at equilibrium, compositions of major elements in addition to the fugitive components can be estimated self consistently in an aqueous phase saturated with the melt for systems at temperatures below the second critical endpoint. This allows the prediction of the compositions of brines evolving from magmatic systems and permits their compositions to be tracked as these systems evolve along a liquid line of descent during solid phase crystallization. Work is in progress to fully integrate these model extensions into the MELTS model collection; the modeling framework will be accessible as a component of the ENKI software ecosystem [4]. To illustrate some model predictions, Figure 1 shows compositions of Cl-brines saturated with five diverse magma types, while Figure 2 shows S redox relations evolving during the closed system crystallization of an olivine tholeiite.

[1] Contrib. Mineral. Petrol. 119:197-212; 169:53, [2] Geochim. Cosmochim. Acta 129:125-45; 254:192-230, [3] Contrib. Mineral. Petrol. 127:176-86; 139:316-25; 154:191-204; 156:785-97 [4] enki-portal.org