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Modeling primordial atmospheric compositions and O_2 abundances from magma ocean and volcanic outgassing with VapoRock

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Silicate vapors play a key role in rocky planet evolution, forming the basis of primordial atmospheres through magma ocean and volcanic outgassing. Interpreting observed atmospheric abundances, like those expected from JWST transit spectroscopy, requires accurate baseline predictions for simple outgassing scenarios (prior to any biotic influence). Atmospheric oxygen abundance represents the largest single leverage point over gas species abundances, given their high sensitivity to oxygen fugacity (fO_2). However, current methods for predicting fO_2 above vaporized silicates rely on the assumption of congruent vaporization, which doesn't hold for many natural outgassing scenarios. To provide accurate outgassing predictions, we present our open-source thermodynamic modeling software "VapoRock" (accepted for publication in the Astrophysical Journal, https://arxiv.org/abs/2208.09582), which combines the MELTS liquid model with JANAF gas-species thermochemical tables. VapoRock calculates abundances of 34 gaseous species in equilibrium with magmatic liquid in the system Si-Mg-Fe-Al-Ca-Na-K-Ti-Cr-O.

Comparison with experiments shows that pressures and melt-oxide activities (which vary by orders of magnitude) are reproduced within a factor of ~3, consistent with measurement uncertainties. We also benchmark our model against a wide selection of igneous rock compositions including bulk silicate Earth, predicting elemental vapor abundances that are comparable (Na, Ca, & Al) or more realistic (K, Si, Mg, Fe, & Ti) than those of the closed-source MAGMA code (Schaefer 2004), with maximum deviations by factors of 10-300 for K & Si. Vapor abundances depend critically on liquid activities, and the MELTS model underpinning VapoRock was calibrated and extensively tested on natural igneous liquids. In contrast, MAGMA's underlying liquid model assumes ideal mixtures of liquid pseudo-species, which only roughly approximates the non-ideal compositional interactions typical of many-component natural silicate melts.

Using VapoRock, we predict outgassed vapor atmospheric abundances for a wide range of natural planetary surface compositions. We additionally demonstrate a new thermodynamically supported method for predicting intrinsic oxygen fugacities---in cases where outgassing dominates the atmospheric redox state---and contrast it with the cation-ratio method employed by other outgassing models like MAGMA. Finally, we explore how relative abundances of SiO and SiO_2 provide a spectroscopically measurable proxy for oxygen fugacity in devolatilized exoplanetary atmospheres, potentially constraining fO_2 in outgassed exoplanetary mantles.