Optical constants of synthetic potassium, sodium, and hydronium jarosite†

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ABSTRACT

The hydroxy sulfate jarosite [(K,Na,H2O)Fe3(SO4)2(OH)6] has both been discovered on Mars, and is associated with areas of highly acidic runoff on Earth. Because jarosite is extremely sensitive to formation conditions, it is an important target mineral for remote sensing applications. Yet at visible and near infrared (VNIR) wavelengths, where many spacecraft spectrometers collect data, the spectral abundance of a mineral in a mixture is not linearly correlated with the surface abundance of that mineral. Radiative transfer modeling can be used to extract quantitative abundance estimates if the optical constants (the real and imaginary indices of refraction, n and k) for all minerals in the mixture are known. Unfortunately, optical constants for a wide variety of minerals, including sulfates like jarosite, are not available. This is due, in part, to the inherent difficulty in obtaining such data for minerals that tend to crystallize naturally as fine-grained (~10 μm) powders, like many sulfates including jarosite. However, the optical constants of powders can be obtained by inverting the equation of radiative transfer and using it to model laboratory spectra. In this paper, we provide robust n and k data for synthetic potassium, hydronium, and sodium jarosite in the VNIR. We also explicitly describe the calculation procedures (including access to our Matlab code) so that others may obtain optical constants of additional minerals. Expansion of the optical constants library in the VNIR will facilitate the extraction of quantitative mineral abundances, leading to more in-depth evaluations of remote sensing target locations.

Keywords: Jarosite, optical constants, radiative transfer, Hapke, index of refraction, sulfate, Mars, AMD

INTRODUCTION

Jarosite has been the subject of a multitude of studies over the past decade (Bishop and Murad 2005; Frost et al. 2005; Navrotsky et al. 2005; Nomura et al. 2005; Barron et al. 2006; Papike et al. 2007; Cloutis et al. 2008; Madden et al. 2008, 2012; Bell et al. 2010; Norlund et al. 2010; Kula and Baldwin 2011; Pritchett et al. 2012; Zahrai et al. 2013) since its discovery on Mars in 2004 at the Mars Exploration Rover Opportunity landing site at Meridiani Planum (Klingelhoefer et al. 2004). On Earth, this iron hydroxy sulfate [(K,Na,H2O)Fe3(SO4)2(OH)6] occurs primarily as an oxidative weathering product of pyrite-rich sediments associated with acid mine drainage (AMD) (Navrotsky et al. 2005). Therefore, its discovery on Mars suggests a highly acidic formation environment (Bishop et al. 2004). On both Earth and Mars, jarosite’s sensitivity to formation conditions makes it an important environmental indicator. It is, therefore, a key remote sensing target. Visible and near infrared (VNIR) remote sensing has been used to identify and map jarosite on both planets (Swayze et al. 2000; Farrand et al. 2009). However, quantitative abundance estimates cannot be extracted from these data because of a lack of optical constants (the real and imaginary indices of refraction, n and k). The absence of these optical constants from the literature is due, in part, to the inherent difficulty in obtaining such data for minerals that tend to crystallize naturally as fine-grained (~10 μm) powders, like many sulfates including jarosite. Yet once optical constants have been determined, and quantitative mineral abundances obtained, it becomes possible to conduct a more in-depth evaluation of the target location. As additional jarosite-bearing regions are discovered on Mars (Farrand et al. 2009; Roach et al. 2010; Wendt et al. 2011; Sefton-Nash et al. 2012; Sowe et al. 2012), there is a growing need for tools and data that can enhance our interpretations of past martian environments. In the absence of targeted sample return, quantitatively modeled mineral abundances derived from remote sensing data can provide valuable constraints on past fluid compositions, atmospheric conditions, weathering timelines, and sub-surface processes. This will aid in developing a full picture of martian history. To this end, jarosite is a particularly valuable environmental indicator mineral because it is extremely sensitive to environmental conditions. For example, terrestrial jarosite only precipitates under very specific Eh and pH conditions as a supergene deposit (Bigham et al. 1996a, 1996b; Norlund et al. 2010). It also only remains stable under a narrow range of atmospheric and surface conditions (i.e., low surface moisture and low relative humidity (Madden et al. 2004; Papike et al. 2006)). This sensitivity has allowed it to be used as a “stopwatch” for wetting processes on Mars (Madden et al. 2009). Jarosite can

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