SPECTRAL PROPERTIES OF Ca-, Mg- AND Fe-BEARING CARBONATES. J. L. Bishop1 M. D. Lane2, A. J. Brown1, T. Hiroi3, G. A. Swayze4 and J.-F. Lin5, 1SETI Institute & NASA-ARC (Mountain View, CA, jbishop@seti.org), 2Planetary Science Institute, (Tucson, AZ), 3Brown University (Providence, RI), 4USGS (Denver, CO), 5University of Texas at Austin (Austin, TX).

Introduction: Reflectance spectra of several carbonates with variable Ca, Mg and Fe concentrations are presented here. Shifts in the NIR band centers near 2.3, 2.5, 3.4 and 4 µm and the mid-IR fundamental vibrations near 750, 900, 1550 cm−1 (~6.5, 11, 14 µm) are observed as a function of the type of cation present. This study builds on earlier analyses of the spectral properties of carbonates [1,2,3] and seeks to provide spectral data that will enable determination of carbonate chemistry through remote sensing on Mars.

Samples: Carbonates were collected from several sources for this study: calcite ML-C2 (CaCO3) from Durango, Mexico, aragonite (CaCO3) from Somerset, England, dolomite ((Ca,Mg)CO3) from Selasvann, Norway, Fe-dolomite ((Ca,Mg,Fe)CO3) from Angels, Calif., ankerite ((Ca,Mg,Fe)CO3), magnesite (MgCO3) from Brumado, Brazil, siderite (FeCO3) from Nova Scotia, Canada. Some carbonates were also synthesized that contain specific amounts of Mg, Fe and Mn cations [4], including: Synth-1 (Mg 0.995, Fe 0.003, Mn 0.002), Synth-2 (Mg 0.33, Fe 0.65, Mn 0.02), and Synth-3 (Mg 0.06, Fe 0.91, Mn 0.03). When sufficient sample material was available, multiple grain sizes were prepared.

Spectral Measurements: Bidirectional reflectance spectra were measured of particulate samples from 0.3-2.5 µm under ambient conditions. FTIR reflectance spectra were measured of particulate samples from 1-25 or 1-50 µm. Some of these data were reported earlier [5,6]. The near-infrared (NIR) data were processed using a continuum removal procedure [7] to enable comparison of the band centers with changes in compositions. Emissivity spectra were measured from 5-25 µm for some carbonates in this study as well as related samples [3].

Figure 1. Continuum-removed spectra of several carbonates with different compositions. Grey lines are drawn at 2.30, 2.34, 2.5, 2.54, 3.27, 3.42, 3.48, 3.80, 3.93, and 3.97 µm to facilitate comparison of the data.

Figure 2. VNIR spectra of the 45-125 µm size fraction of three synthetic carbonates. The dominant carbonate bands and the Fe band are labeled.

Figure 3. Carbonate band center comparison for the 2.3 and 2.5 µm bands. Values determined from the continuum-removed spectra.
band is similar in shape and intensity for Synth-2 (65% Fe) and Synth-3 (91% Fe). Multiple vibrational absorptions due to CO$_3^{2-}$ are observed from 1.5-5 $\mu$m. Gaffey [1] found that the ~2.3 and 2.5 $\mu$m band centers are coordinated and that these are correlated with the mass of the cation. Band centers for our data are plotted in Figure 3.

Band depths typically increase for increasing particle sizes in the NIR region (Figure 4), except for the band near 4 $\mu$m, likely due to saturation. Particle size also influences the band shape and changes the spectral properties sufficiently in some cases that it could influence detection of these minerals.

Mid-IR Spectral Analyses: Three dominant bands are observed for carbonates in the mid-IR region. These include the asymmetric stretching vibration (v3), the out-of-plane bending vibration (v2) and the in-plane bending vibration (v1) [3,8]. These are observed near 1525, 885 and 710 cm$^{-1}$ for calcite (Figure 5) and near 1560, 890 and 750 cm$^{-1}$ for Fe/Mg-carbonate (Figure 6). The bending vibrations for carbonates are particularly sensitive to grain size and flip from bands to peaks for smaller particles [9].

Applications: Fe/Mg-carbonate has been proposed as a type of carbonate on Mars [e.g. 10-11]. Other studies using CRISM data have proposed Mg- and Ca-bearing carbonates [e.g. 12-16] and potentially talc-carbonation of serpentine [13,16]. Studying the spectral properties of carbonates as a function of cation composition and grain size will facilitate characterization of carbonates on Mars. Another motivation for characterizing Fe/Mg-carbonates is that they are thought to be a host mineral of carbon in the Earth’s mantle [4].

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