1 **REVISION 2**

2 Mid-infrared optical constants of clinopyroxene and orthoclase derived from oriented single-

3 crystal reflectance spectra

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6 **Abstract**

7 We have determined the mid-IR optical constants of one alkali feldspar and four pyroxene

8 compositions in the range of 250–4000 cm^{-1}. Measured reflectance spectra of oriented single crystals

9 were iteratively fit to modeled spectra derived from classical dispersion analysis. We present the real

10 and imaginary indices of refraction (*n* and *k*) along with the oscillator parameters with which they were

11 modeled. While materials of orthorhombic symmetry and higher are well-covered by the current

12 literature, optical constants have been derived for only a handful of geologically relevant monoclinic

13 materials, including gypsum and orthoclase. Two input parameters that go into radiative transfer

14 models, the scattering phase function and the single scattering albedo, are functions of a material's

15 optical constants. Pyroxene is a common rock-forming mineral group in terrestrial bodies as well

16 meteorites and is also detected in cosmic dust. Hence, having a set of pyroxene optical constants will

17 provide additional details about the composition of solar system bodies and circumstellar materials. We

18 follow the method of Mayerhofer et al. (2010), which is based on the Berreman 4x4 matrix

19 formulation. This approach provides a consistent way to calculate the reflectance coefficients in low-

20 symmetry cases. Additionally, while many models assume normal incidence to simplify the dispersion

21 relations, this more general model applies to reflectance spectra collected at non-normal incidence.

22 **1. Introduction**

23   Pyroxenes are common rock-forming minerals in terrestrial planets and asteroids. They are also

24   abundant in meteorites and interplanetary and cosmic dust particles. The pyroxene crystal structure

25   allows for a variety of cations to occupy its M1 and M2 sites, with ordering and preference between the

26   two sites being controlled by temperature, pressure, and cooling rate. As a result, pyroxene composition

27   is a good indicator of the thermal history of the source magma (Kilma et al. 2008) and can be used to

28   compare the evolution of different planetary bodies (Karner et al. 2006). Pyroxene is readily detected in

29   the near-infrared (NIR) via two strong $Fe^{2\cdot}$ crystal field absorption bands near 1 and 2 μm whose

30   positions and strengths are functions of composition. As the mid-IR (MIR, around 3-15 μm, though

31   definitions vary) is sensitive to Si–O vibrational modes (Salisbury 1972), it can be used to provide

32   additional details about composition as well as to estimate abundance relative to more felsic

33   components (Ramsey and Christensen 1998).

34   The wavelength-dependent complex index of refraction ($\tilde{n}=n+ik$), where n and k are the optical

35   constants, is an essential input into scattering models of planetary surfaces. Commonly used radiative

36   transfer models of airless bodies include Lumme and Bowell (1981), Hapke (1993a, 2012), Shkuratov

37   et al. (1999) and Mishchenko et al. (1999). Hapke's theory uses optical constants to calculate the single

38   scattering albedo and the phase function. In Skhuratov's model of lunar regolith scattering, the

39   reflectance of the surface (A) is dependent on only four parameters $A(n,k,S,q)$, where n and k are the

40   optical constants, S is the scattering path-length and q is the packing density (Skhuratov et al. 1999).

41   Hence, accurate determination of optical constants for a variety of minerals is necessary for using

42   remote sensing data to make quantitative estimates of mineralogical composition. At MIR wavelengths,

43   materials of orthorhombic symmetry and higher are well-covered by the current literature; these

44   include quartz, calcite, olivine, orthopyroxene, kaolinite, serpentine, palagonite, and iron oxides

45   (Spitzer and Kleinman 1961; Wenrich and Christensen 1996; Lucy 1998; Lane 1999; Suto et al. 2002;

46   Glotch et al. 2006; Sogawa et al. 2006; Dyar et al. 2009; Roush et al.1991; Glotch and Rossman 2009).

47   Monoclinic and triclinic minerals have largely been ignored in optical constant research,

48   although in some cases orientation-averaged effective optical constants have been calculated and

49   presented (e.g., Roush et al. 1991; Glotch et al. 2007). This is due to the additional complexity of

50   obtaining values for low-symmetry materials, despite the fact that these crystal systems contain

51   important rock-forming mineral groups such as clinopyroxene and feldspar. In this work, we use

52   dispersion analysis to calculate the optical constants of four distinct clinopyroxene compositions in the

53   range of $250–4000$ cm^{-1}, following the method of Mayerhofer et al. (2010) and present a procedure that

54   can be applied to derive the optical constants of monoclinic single crystals. We also calculate the

55   optical constants of orthoclase and compare to the previously computed optical constants of Aronson

56   (1986) as a test of our model.

57   **2. Background**

58   *2.1 The Moon*

59   The Clementine mission provided a global lunar map of pyroxene abundance, broadly

60   highlighting that it is a major component of the mare basalts and less prevalent in highlands. Modeled

61   clinopyroxene concentrations are especially high in fresh mare craters due the short exposure ages of

62   these surfaces (Shkuratov et al. 2004). While pyroxene is only a minor component in the lunar

63   highlands it is found in the following highlands rock types: ferroan anorthosites (FAN's), alkali- and

64   Mg-suite rocks (Tompkins and Pieters 1999). Attempting to put these in a global context, Klima et al.

65   (2011) used NIR data from the Moon Mineralogy Mapper (M^3) to detail the distribution of high– vs.

66   low-Ca pyroxene and estimate Mg #. Low-Ca pyroxene is limited to regional exposures within the

67   South Pole-Aitken Basin and in the highlands north and south of Mare Frigoris, approximately half of

68   which have Mg # (Mg/(Mg+Fe)) commensurate with FAN rocks (~Mg # $55–75$).

69   MIR emission data from the Diviner Lunar Radiometer Experiment complements visible near-

70   IR (VNIR) measurements from Clementine and M^3, as they are able to detect Fe-poor lithologies in the

71 presence of mafic materials such as pyroxene and olivine. Three of Diviner's channels are centered near

72 the silicate Christiansen feature (CF) (Paige et al. 2010), which is an emissivity maximum whose

73 position moves to shorter wavelengths with increasing SiO_2 polymerization (Conel 1969; Logan et al.

74 1973; Salisbury and Walter 1989), allowing Diviner to be used to map silicate compositions across the

75 Moon (Greenhagen et al. 2010; Glotch et al. 2010, 2011; Song et al. 2013; Allen et al. 2011; Arnold et

76 al. 2013). A global map of CF position clearly demonstrates the difference between the relatively

77 pyroxene-rich mare and feldspar-rich highlands (Greenhagen et al. 2010). Although Diviner has only

78 three spectral bands in the 8 μm range, laboratory measurements in a simulated lunar environment

79 show the estimated CF position combined with spectral shape is adequate to distinguish pyroxene from

80 a mixture of plagioclase and olivine (Donaldson Hanna et al. 2012).

81 *2.2 Mars*

82 The low-albedo regions of Mars were initially categorized into two surface compositions based

83 on Mars Global Surveryor Thermal Emission Spectrometer (MGS-TES) data, where Surface Type 1

84 was determined to be basalt containing ~25% clinopyroxene (Bandfield et al 2000, Hamilton et al.

85 2001). Rogers et al. (2007) defined 4 distinct spectral types within low-albedo terrains. Subsequently,

86 Rogers and Christensen (2007) determined the mineralogy of these four groups, with clinopyroxene

87 abundance being one of the major distinguishing features. While low-Ca pyroxenes were mostly

88 detected in Noachian terrain, high-Ca pyroxene was found in a wider age-range of units. Some of the

89 mineralogical differences between the four groups, especially high silica phases, are the result of

90 weathering. However, the differences in pyroxene abundance likely represent differences in the magma

91 from which the crust was derived. These differences were also identified with data from the OMEGA

92 (Observatoire pour la Minéralogie, l'Eau, les Glaces et l'Activité) NIR imaging spectrometer. Using

93 this instrument, Ody et al. (2012) presented global maps of anhydrous minerals, including pyroxene.

94 The highest pyroxene concentration occurs in the Syrtis Major volcanic province, which is coincident

95 with Group 2 of Rogers and Christensen (2007). Glotch and Rogers (2013) suggested that the unusually

96   high concentration of high-Ca pyroxene at this site was the result of subsurface interactions of basaltic

97   magma and a Ca-carbonate-bearing layer.

98   *2.3 Asteroids*

99   Pyroxene has been identified in several S-type asteroid families (Chapman et al. 1975).

100   Sunshine et al. (2004) applied the Modified Gaussian Model (MGM) to VNIR asteroid spectra

101   collected by the NASA Infrared Telescope Facility (IRTF), to determine the relative amounts of low-

102   and high calcium pyroxene. They determined that the Vestoids and well as the S-type asteroid families

103   Merxia and Agnia have a high ratio of high calcium pyroxene to total pyroxene, indicating that they are

104   derived from differentiated bodies.

105   Pyroxene absorptions are the most common VNIR spectral feature on the surface of the asteroid

106   Vesta, which was first linked to the HED (howardite-eucrite-diogenite) meteorites due to the similarity

107   of their 0.9 μm band in VNIR spectra (McCord et al. 1970). The findings of Dawn's Visible InfraRed

108   (VIR) mapping spectrometer support this connection. Much of the surface shows a howardite-like

109   spectrum intermixed with smaller-scale regions resembling eucrites and diogenites. The south polar

110   region (Rheasilvia), a large impact basin, is consistent with more Mg-rich pyroxene characteristic of

111   diogenites (De Sanctis et al. 2012). These spectral variations are indicative of a differentiated crust

112   where the deeper diogenitic materials have been exposed through impact.

113   *2.4 Interplanetary and Interstellar Dust*

114   The presence of crystalline silicates in interplanetary dust particles (IDPs) was established

115   through micrometeorite samples collected from Earth's stratosphere (Bradley et al. 1983, Mackinnon

116   and Rietmeijer 1987). Additionally, ground-based MIR spectra from three different instruments

117   provided evidence for crystalline silicates in comets (Hanner et al. 1994). Prior to the Infrared Space

118   Observatory (ISO), whose instruments covered a range of ~2.5 – 240 μm, silicates in cosmic dust were

119   thought to be primarily amorphous (Roush et al. 1991; Molster and Kemper 2004). This assumption

120   guided most previous laboratory studies of pyroxene optical constants (Jäger et al. 1994; Dorschner et

121   al. 1995; Henning and Mutschke 1997). Using ISO, crystalline pyroxene was detected in dust produced

122   by evolved stars (Molster et al. 2002), the circumstellar disks of young stellar objects (YSO's)

123   (Bouwman et al. 2001) and planetary nebula (Beintema 1997). As a result of the detection of crystalline

124   pyroxene around planetary nebula, Jäger et al. (1998) estimated the MIR optical constants for a natural

125   enstatite (low-Ca orthopyroxene) sample along the crystallographic axes using Kramers-Kronig

126   analysis. Better characterization of the materials in circumstellar environments would improve our

127   understanding of dust formation and processing and enable comparison to our own solar system.

128   **3. Methods**

129   3.1 *Sample description and preparation*

130   All samples are large single crystals (roughly 0.5–1 cm on a side) and their chemical

131   compositions are summarized in Table 1. The major element abundances were determined by scanning

132   electron microscope energy dispersive x-ray spectroscopy (SEM–EDS). To produce the chemical

133   formulas in Table 1, atomic abundances of oxygen were assumed by stoichiometry to be O_6, which

134   may introduce error if any non-pyroxene phases are present in the samples. We prepared thin sections

135   of each sample in order to optically examine the samples for exsolution and twinning. One augite

136   (Aug1) sample was loaned from the Stony Brook Geosciences Department mineral collection and

137   originates from Indian Well, AZ. This sample does not show signs of exsolution or twinning. The

138   diopside (Diop1) sample was purchased from Kelly's Rocks and is from Magog, QC, Canada. While

139   twinning is present over ~30–40% of a section perpendicular to the *a-c* plane in the diopside sample,

140   the IR spectra match previously published oriented reflectance spectra (Johnson et al. 2002). The

141   hedenbergite (Hed1) and second augite (Aug2) sample were provided by D. Lindsley at Stony Brook

142   University. The hedenbergite sample does not exhibit exsolution or twinning, while Aug2 appears to

143   contain lamellae that remain dark under crossed polar illumination at all orientations. Micro-FTIR

144   spectra of these lamellae are quite noisy compared to the rest of the augite sample, and show a broad

145   reflectance peak at around 3900 cm^{-1} and a peak at 1015cm^{-1}. These spectral features indicate some

146   type of clay, however the exact composition is difficult to discern. The FITR spectrum of the whole

147   sample does not show a 3900 cm^{-1} peak, indicating this is a relatively minor component. The diopside,

148   hedenbergite, and augite compositions are shown on the ternary diagram in Figure 1. We cut each

149   sample with a diamond saw blade so that one surface is parallel to the *a-c* plane (010) and the other

150   perpendicular to it –– planes (001) or (100). We polished these surfaces to 0.25 μm surface roughness,

151   and confirmed the orientations of the cut surfaces by single crystal XRD. XRD analysis involved

152   collection of the preliminary set of frames (pre-experiment) for the determination of unit cell and the

153   orientation matrix. Using this information, we indexed the faces of the crystal with the CrysAlisPRO

154   software. We collected reflections for determination of the orientation matrix using a four-circle kappa

155   Oxford Gemini diffractometer equipped with an Atlas detector ($\lambda = 0.71073$ Å).

156   *3.2 Collection of mid and far-IR reflectance spectra*

157   We acquired specular reflectance spectra on the Stony Brook University Vibrational

158   Spectroscopy Laboratory's Nicolet 6700 Fourier Transform Infrared (FTIR) spectrometer using a

159   FT–30 specular reflectance accessory with incidence and reflection angles of 30 degrees at a spectral

160   sampling of 2 cm^{-1}. An InfraSpecs wire grid IR polarizer was placed in the beam path for collection of

161   polarized reflectance spectra. For each sample, we measured reflectance spectra for four orientations of

162   the crystal with respect to the incident polarized beam. Depending on whether the *a*– or *c*–axis was

163   more readily identifiable, these orientations were 0°, 45°, 90° and 110° from the identified

164   crystallographic axis. MIR spectra were collected over a range of 400–4000 cm^{-1} using a KBr

165   beamsplitter and DTGS detector with a CsI window. Each spectrum is an average of 256 scans. Far-IR

166   (FIR) spectra were acquired from 250–600 cm^{-1} using a Nicolet Solid Substrate beamsplitter and a

167   DTGS detector with a polyethylene window. Each of these spectra is an average of 512 scans. The two

168   wavelength ranges are joined at 600 cm^{-1} using the overlapping region (600 cm^{-1} – 400 cm^{-1}) to scale

169   the spectral contrast of the FIR spectra. MIR and FIR spectral contrast varies by up to 10% due to slight

170   differences in measurement conditions and/or a few degree error in crystal orientation. Samples were

171   placed on a holder that acts as a mask, controlling the spot size. We chose the largest spot size that can

172   be completely covered by the polished surface of the sample. The bottom of the sample holders is

173   coated with paraffin soot to reduce stray reflectance off of the holder into the sample chamber. For the

174   smaller spot-sizes (<0.5 cm diameter) we subtracted a spectrum of the sample holder without a sample

175   or standard placed on top. While the sample holder does not affect the mid-IR reflectance, there is a

176   steep upward slope starting at around 400 cm^{-1} which rapidly increases from 0.01 to several percent

177   reflectance at ~100 cm^{-1}.

178   *3.3 Modeling of optical constants*

179   The optical constants (*n,k*) are related to the wavelength-dependent dielectric function ($\varepsilon(\lambda)$) of

180   the material ($\tilde{n} = \varepsilon^{1/2}$). Electron states in non-conducting materials can be modeled as damped harmonic

181   oscillators, which exhibit spring-like behavior (Griffiths 1999). The E-field of the incoming beam acts

182   as a driving force on the oscillators, which have resonant frequencies ν_j (cm^{-1}). The parameters s_j (cm^{-}

183   ^{2}), γ_j (cm^{-1}) and ε_∞ are the oscillator strength, damping coefficient (proportional to the oscillator

184   velocity) and infinite frequency dielectric constant respectively. These parameters are explained in

185   more detail in section 5.1.

186   For minerals of orthorhombic and higher symmetry, we can assume that these oscillations occur

187   parallel to the crystallographic axes. In this case, optical constants can be determined using the

188   approach of Spitzer and Kleinman (1961). Reflectance spectra are acquired for each principal axis with

189   the polarization parallel to each axis. Each spectrum is iteratively fit with estimated values of the

190   oscillator parameters as input.

191   When a mineral is biaxial and the axes are not orthogonal, the oscillators cannot be assumed to

192   be parallel to the crystallographic axes (Belousov and Pavinich 1978). In a monoclinic material, optical

193   constants with E parallel to the *b*-axis (where the oscillators are parallel to the axis) can be determined

194   in the same manner as the orthorhombic case. In the *a−c* plane, oscillators are coplanar with, but not

195   parallel to the crystallographic axes. To determine the two remaining principle refractive indices, it is

196   necessary to make measurements at three different angles (Ω) with respect to the crystallographic axes

197   in the *a-c* plane (Aronson et al. 1983), with measurements at more angles providing more robust fits.

198   This results in an additional oscillator parameters θ_j and φ_j. A useful diagram of such an experimental

199   setup is given in Fig. 1 of Ivanovski et al. (2007). The principle complex indices of refraction are the

200   eigenvalues of the complex dielectric-permittivity tensor, which can be calculated as follows, where N

201   is the number of oscillators:

202
$$E = (n + ik)^2 = \begin{pmatrix} \varepsilon_{\infty xx} & \varepsilon_{\infty xy} & \varepsilon_{\infty xz} \\ \varepsilon_{\infty yx} & \varepsilon_{\infty yy} & \varepsilon_{\infty yz} \\ \varepsilon_{\infty zx} & \varepsilon_{\infty zy} & \varepsilon_{\infty zz} \end{pmatrix} + \sum_{j=1}^{N} \frac{s_j}{v_j^2 - i\gamma_j v - v^2} \times$$

203
$$\begin{pmatrix} \sin^2\theta_j\cos^2\varphi_j & \sin^2\theta_j\sin\varphi_j\cos\varphi_j & \sin\theta_j\cos\theta_j\cos\varphi_j \\ \sin^2\theta_j\sin\varphi_j\cos\varphi_j & \sin^2\theta_j\sin^2\varphi_j & \sin\theta_j\cos\theta_j\sin\varphi_j \\ \sin\theta_j\cos\theta_j\cos\varphi_j & \sin\theta_j\cos\theta_j\sin\varphi_j & \cos^2\theta_j \end{pmatrix} \qquad (1)$$

204

205   The reflectance spectra for all Ω are fit simultaneously. Fixing the *b*-axis as the *z*-axis of the

206   dielectric tensor, ε needs to be rotated with Ω, according to:

207
$$\varepsilon = \begin{pmatrix} \cos\Omega & \sin\Omega \\ -\sin\Omega & \cos\Omega \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} \\ \varepsilon_{xy} & \varepsilon_{zz} \end{pmatrix} \begin{pmatrix} \cos\Omega & -\sin\Omega \\ \sin\Omega & \cos\Omega \end{pmatrix} \qquad (2)$$

208
209   Because of the additional complexity in measurement and calculation, optical constants have

210   been derived from single crystal samples for only a few monoclinic materials, including gypsum and

211   orthoclase (Long et al.1992; Aronson et al. 1983, Aronson 1986). A similar method for triclinic

212   materials is outlined by Aronson et al. (1985). However, substitution of the relevant variables in their

213   equations for the reflection coefficients results in a singularity for the monoclinic case (Mayerhofer et

214 al. 2010) instead of reducing to the formulas given in Aronson et al. (1983). In addition, Aronson et

215 al.'s formulation applies only to the case of normal incidence. The Berreman 4x4 matrix formulation

216 (Berreman 1972) gives a more consistent approach for calculating the reflectance coefficients in low-

217 symmetry cases (Mayerhofer and Popp 2007).

218   Mayerhofer and Popp (2007) define a matrix $\widetilde{M}$ that can be used to calculate the reflection

219 coefficients as a function of incidence angle (α):

220      $$\widetilde{M} = D_\Psi^{-1}(0)D_\Psi(1) \tag{3}$$

221      $$r_{xx} = \frac{\widetilde{M}_{21}\widetilde{M}_{33} - \widetilde{M}_{23}\widetilde{M}_{31}}{\widetilde{M}_{11}\widetilde{M}_{33} - \widetilde{M}_{13}\widetilde{M}_{31}} \tag{4a}$$

222      $$r_{xy} = \frac{\widetilde{M}_{41}\widetilde{M}_{33} - \widetilde{M}_{43}\widetilde{M}_{31}}{\widetilde{M}_{11}\widetilde{M}_{33} - \widetilde{M}_{13}\widetilde{M}_{31}} \tag{4b}$$

223 $D\Psi(0)$ and $D\Psi(1)$ are the dynamical matrices of the incident and refracted waves (Yeh 1979):

224      $$D_\Psi^{-1}(0) = \frac{1}{2}\begin{pmatrix} 1 & 1/ncos\alpha & 0 & 0 \\ 1 & -1/ncos\alpha & 0 & 0 \\ 0 & 0 & 1/cos\alpha & 1/n \\ 0 & 0 & -1/cos\alpha & 1/n \end{pmatrix} \tag{5}$$

225

226      $$D_\Psi(1) = \begin{pmatrix} \varepsilon_{xy}(1-\frac{k_y^2}{\varepsilon_{zz}}) & 0 & \varepsilon_{xy}(1-\frac{k_y^2}{\varepsilon_{zz}}) & 0 \\ \mathring{a}_{xy}(1-\frac{k_y^2}{\varepsilon_{zz}})\gamma_1 & 0 & \varepsilon_{xy}(1-\frac{k_y^2}{\varepsilon_{zz}})\gamma_3 & 0 \\ (1-\frac{k_y^2}{\varepsilon_{zz}})[\gamma_1^2 - (\varepsilon_{xx} - k_y^2)] & 0 & (1-\frac{k_y^2}{\varepsilon_{zz}})[\gamma_3^2 - (\varepsilon_{xx} - k_y^2)] & 0 \\ [\gamma_1^2 - (\varepsilon_{xx} - k_y^2)]\gamma_1 & 0 & [\gamma_3^2 - (\varepsilon_{xx} - k_y^2)]\gamma_3 & 0 \end{pmatrix} \tag{6}$$

227 where n is the index of refraction of the incident medium, k_y is the y-component of the wave-vector (the

228 magnitude and direction of the incoming beam), and

229      $$\gamma_1 = \sqrt{-\frac{1}{2\varepsilon_{zz}}(K_1 + \sqrt{K_1^2 + K_2})} \tag{7a}$$

230      $$\gamma_3 = \sqrt{\frac{1}{\varepsilon_{zz}}(-K_1 + \sqrt{K_1^2 + K_2})} \tag{7b}$$

231      $$K_1 = -\varepsilon_{zz}(\varepsilon_{xx} + \varepsilon_{yy}) + k_y^2(\varepsilon_{yy} + \varepsilon_{zz}) \tag{8a}$$

232    $$K_2 = -4 \left[\varepsilon_{xy}^2 + \varepsilon_{yy} \left(k_y^2 - \varepsilon_{xx} \right) \right] (k_y^2 - \varepsilon_{zz}) \varepsilon_{zz}. \tag{8b}$$

233   To perform the required calculations, we use the Matlab non-linear fitting routine lsqcurvefit,

234   which allows us to set lower and upper bounds, ensuring that the final values for the oscillator

235   parameters are positive. To produce the initial parameters for this model, we first fit the spectrum for

236   each Ω as if it is orthorhombic and at normal incidence. The parameters ν_j and γ_j can be estimated

237   reasonably by visual inspection, while s_j is estimated as in Pavinich and Belousov (1978). Reflectance

238   spectra for all orientations are then fit simultaneously, using the Ω where s_j is the largest for a given ν_j

239   as an initial guess for φ_j.

240   We attempt to fit the reflectance spectrum with the minimum number of oscillators necessary.

241   Starting with the number of main peaks, modes are added until a reasonable fit is obtained for any

242   overlapping peaks or shoulders (a difference between the measured and modeled reflectance of less

243   than 10%). Sometimes modes can be at the same frequency or very close in frequency, with different

244   θ_j. In this case, although there is only one peak, the fit will be poor without an additional oscillator.

245   *3.4 Oscillator parameter error estimates*

246   The model fit is commonly assessed using the standard error of the oscillator parameters. We

247   report the standard error ($\sigma(\nu)$, $\sigma(\gamma)$ etc.) for each parameter in Tables 2-6. This does not reflect the

248   impact of the initial guesses of the oscillator parameters on the final reflectance fit. Poor initial

249   estimates of starting values may result in slow convergence, non-convergence or convergence on a

250   local rather than global minimum in our model. For each sample, we used five different sets of starting

251   values centered around those produced by the fit to the orthorhombic model to qualitatively evaluate

252   how much the final *n* and *k* values depended on the initial estimates. Those that gave the best

253   reflectance fit were used to calculate the optical constants. As an additional test, we independently

254   varied the sets of ν_j , γ_j, s_j, and φ_j parameters for a gem-quality orthoclase sample to determine which

255   had the largest impact on the final *n* and *k* values. Large ($\pm$ 30 cm^{-1} for ν_j and $\pm$ 50% for all others)

256   variations in the other parameters do not appear to have a major effect on the fit (see Figures 2–5).

257   Figure 6 shows the final fits when all parameters are varied by these amounts (top) as well the 95%

258   confidence bounds based of the standard error of the parameters (bottom). The two measures of

259   uncertainty appear to diverge from the calculated optical constants at different wavenumbers.

260

261   **4. Results**

262   For each sample we present the measured and modeled reflectance and the plots of n and k as a

263   function of wavelength derived from the reflectance fit. The measured and modeled spectra, as well as

264   the   derived   optical   constants   and   oscillator   parameters   are   available   at

265   http://aram.ess.sunysb.edu/tglotch/optical_constants.html.

266   *4.1 Augite 1*

267   Measured reflectance and model are shown in Figure 7, with incident E-field polarization parallel to the

268   *a-c* plane (top three) and parallel to b (bottom). Derived values of n and k are shown in Figure 8. In

269   Figure 8 n1, n2 and k1, k2 are the optical constants for the rays whose polarization direction is parallel

270   to the *a-c* plane, while nb and kb are the optical constants for the rays with polarization direction along

271   the b crystallographic axis. Oscillator parameters for this sample are given in Table 2.

272   *4.2 Augite 2*

273   Measured reflectance and model are shown in Figure 9, with incident E-field polarization parallel to the

274   *a-c* plane (top three) and parallel to b (bottom). Derived values of n and k are given in Figure 10. In

275   Figure 10 n1, n2 and k1, k2 are the optical constants for the rays whose polarization direction is parallel

276   to the *a-c* plane, while nb and kb are the optical constants for the rays with polarization direction along

277   the b crystallographic axis. Oscillator parameters for this sample are given in Table 3.

278   *4.3 Diopside*

279   Measured reflectance and model are shown in Figure 11, with incident E-field polarization parallel to

280   the *a-c* plane (top three) and parallel to b (bottom). Derived values of n and k are shown in Figure 12.

281   In Figure 12 n1, n2 and k1, k2 are the optical constants for the rays whose polarization direction is

282   parallel to the *a-c* plane, while nb and kb are the optical constants for the rays with polarization

283   direction along the b crystallographic axis. Oscillator parameters for this sample are given in Table 4.

284   *4.4 Hedenbergite*

285   Measured reflectance and model are shown in Figure 13, with incident E-field polarization parallel to

286   the *a-c* plane (top three) and parallel to b (bottom). Derived values of *n* and *k* are shown in Figure 14.

287   In Figure 14 n1, n2 and k1, k2 are the optical constants for the rays whose polarization direction is

288   parallel to the *a-c* plane, while nb and kb are the optical constants for the rays with polarization

289   direction along the b crystallographic axis.Oscillator parameters for this sample are given in Table 5.

290   *4.5 Orthoclase*

291   Measured reflectance and model are shown in Figure 15, with incident E-field polarization parallel to

292   the *a-c* plane (top three) and parallel to b (bottom). Derived values of *n* and *k* are shown in Figure 16 as

293   well as those from Aronson et al. (1986). In Figure 16 n1, n2 and k1, k2 are the optical constants for

294   the rays whose polarization direction is parallel to the a-c plane, while nb and kb are the optical

295   constants for the rays with polarization direction along the b crystallographic axis. Oscillator

296   parameters for this sample are given in Table 6.

297

298   **5. Discussion**

299   *5.1 Interpretation of dispersion parameters*

300   The optical constants n and k are related to the polarizability (α), the dependence of the

301   magnitude of the dipole moment on an applied electric field, and conductivity (σ), the ability of a

302   material to carry a current, which are both properties of the material. The dependence of the

303   polarizability and conductivity and hence the optical constants on wavelength are given by dispersion

304   relations. To derive these dispersion relations, Lorentz postulated that insulating materials contain

305   electrons that are bound to atoms or molecules by Hooke's law forces (Seitz 1940), so that the binding

306   force is proportional to the charge displacement. The motion of the bound electron is described as a

307   harmonic oscillator subject to a periodic electric field ($\mathbf{E}=\mathbf{E_o}e^{-2\pi i\nu t)}$) and damped by a force proportional

308   to the electron's velocity ($m_e\gamma$ (∗note to editor the following should be in line∗)
$$\frac{dx}{dt}$$

309   ) giving: (∗end line∗)

310     $$\frac{d^2x}{d^2t} + 2\pi\gamma\frac{dx}{dt} + 4\pi^2\nu_0^2x = \frac{-q_e}{m_e}E_0e^{2\pi i\nu t} \qquad (9)$$

311     $$x = \frac{q_e}{4\pi^2 m_e}\frac{E_0e^{-2\pi i\nu t}}{\nu_0^2 - \nu^2 - i\gamma\nu} \qquad (10)$$

312   The resonant frequency of the oscillator is ν_0 and the damping constant is $2\pi m_e \gamma$. As ν passes through

313   the value ν_0, there is a peak in the absorption coefficient with a half-width of roughly γ. The order of

314   magnitude of γ can be estimated by the following (Seitz 1940):

315   $$\gamma \sim \frac{4\pi\nu^2 q_e^2}{3m_e c}$$ (11)

316   Where q_e is in statcoulombs, ν is in wavenumbers, m_e is in grams and c is in cm/s. Looking at Eq (10)

317   and assuming the dipole moment has a linear response to the electric field (**p**=$\varepsilon_0\alpha$**E**), results in:

318   $$\alpha = \frac{q_e^2}{4\pi^2 m_e \varepsilon_0} \frac{1}{\nu_0^2 - \nu^2 - i\gamma\nu}$$ (12)

319   Using a form of the Clausius-Mosotti relation $\varepsilon = \varepsilon_\infty + 4\pi\chi = \varepsilon_\infty + 4\pi N\alpha$ (Spitzer et al. 1959) gives the

320   dispersion relation for a single resonance.

321   Of course, for a given material, there will not be just one resonant frequency, but several ν_j each

322   with a different damping constant γ_j. The quantum mechanical approach to this problem deals with this

323   and also gives one additional parameter oscillator "strength" (f_j), a weighting for each oscillator that

324   relates to the absorption or transition probability (Seitz 1940; Spitzer and Kleinman 1961; Born and

325   Wolf 1970). The parameter s_j used in Eq (1) can be defined in terms of f_j as shown in Spitzer and

326   Kleinman (1961).

327   $$s_j = 4\pi\rho_j\nu_j^2 = \frac{Nq_e^2}{\pi m_e} f_j$$ (13)

328   While educated guesses can be made, the oscillator parameters (ν_j, γ_j, and s_j) are difficult to

329   derive exactly from first principles, which is why an iterative technique is normally used. The infinite

330   frequency dielectric constant ε_∞ can be estimated from the square of the visible-wavelength index of

331   refraction (Roush et al. 1991).

332   *5.2 Comparison with previously derived Orthoclase optical constants*

333   Optical constants for orthoclase have been derived from oriented single crystal reflectance

334   spectra by previous workers (Aronson et al. 1986). Figure 16 shows the values found in this study

335   along with those from Aronson et al. (1986). The optical constants for the E-field polarization parallel

336   to b orientation (nb and kb) are very similar, while the optical constants (n1,n2 and k1,k2) for the E-

337   field parallel to the *a-c* plane have slight differences. Variations between the two data sets may be due

338   to either compositional differences in the samples or uncertainties in orientation. Our orthoclase sample

339   had a small amount of Fe^{3+} substituting for Al^{3+} (see Table 1). However, without any compositional

340   information on the sample used in the Aronson et al. (1986) study, it is difficult to make inferences

341   about specific bands.

342   5.3 *Dependence of optical constants on crystal structure and chemistry*

343   Isometric minerals will have one set of optical constants for each wavelength. Because most

344   minerals are anisotropic, the polarizability and conductivity will be directionally as well as wavelength

345   dependent and therefore so will the optical constants. Dispersion in uniaxial and biaxial minerals is

346   described by a dielectric tensor rather than just a dielectric constant. The number of oscillator

347   parameters necessary to fit the reflectance spectrum generally increases with decreasing crystal

348   symmetry. Figure 17 shows averaged optical constants in the MIR for several minerals that belong to

349   different crystal systems. It is also important to measure optical constants for several different chemical

350   compositions within the same mineral group. As shown in this work, optical constants vary

351   considerably with chemistry. Simply using one composition of olivine, for example, may produce poor

352   fits for mineralogical abundance as shown in Liu (2012) at VNIR wavelengths.

353   For silicates, there is a steep absorption edge in the UV-range after which *k*-values drop by

354   orders of magnitude and remain low through the VNIR. As a result, after the UV-edge, dispersion is

355   low until the MIR, where the fundamental vibrational bands occur. There is a steep rise in *k* between 8

356   and 10 μm (1250cm^{-1}–1000cm^{-1}), with the maximum *k* occurring where *n*=1 or slightly lower than 1.

357   This is known as the Christiansen feature and is associated with a minimum in reflectance and a

358   maximum in emission. This feature is the means by which Diviner data are used to identify lunar

359   silicates (Greenhagen et al. 2010). Following the Christiansen feature, there is a steep drop-off in *k* and

360   rise in *n*, causing a drop-off in emission followed by Reststrahlen features. For pyroxenes, spectral

361   features in the ~8–22 μm (~1250cm^{-1}–450cm^{-1}) range are mainly due to Si–O stretching, Si–O–Si

362   bending and modes of the cation-O$_6$ octahedra. The positions of absorptions at these wavelengths vary

363   with Mg # (defined as Mg/(Mg+Fe)) (Jäger et al. 1998; Hamilton 2000; Bowey et al. 2007; Lane et al.

364   2011), likely due to the effect of the substitution on the octahedral layer, which in turn alters the Si-O

365   vibrations (Hamilton 2000; Klima 2007). To demonstrate these effects, Figure 18 shows the reflectance

366   and optical constants for olivine (from Zeidler et al. 2011) ranging from the UV through the MIR, with

367   the major spectroscopic features labeled. This figure also demonstrates that n and k values of silicates

368   vary considerably in the mid-IR as compared with other wavelengths.

369   Amorphous pyroxenes produced by vapor phase condensation and synthetic glasses of pyroxene

370   composition will lack many of the spectroscopic features of a crystalline pyroxene. As a result, the

371   optical constants of these materials will have broader and fewer peaks than crystalline pyroxene. To

372   date, little work has been done on oriented crystalline samples (Jäger et al. 1998), and none has been

373   done to date on clinopyroxene. Figure 19 demonstrates the difference between optical constants of

374   crystalline vs. amorphous phases. Additionally, oriented single crystal spectra are preferable to

375   orientation-averaged data acquired from pellets pressed from powders, as the lower maxima of the

376   specular reflectance peaks of pellets results in lower maxima of derived optical constants when

377   compared to orientation-averaged single crystal optical constants (Roush 1991).

378

379   **6. Implications**

380   Radiative transfer models of planetary surfaces require optical constants for each component

381   that may be present. Applying these models is difficult in the MIR due to the absence of optical

382   constants for many important minerals in the monoclinic and triclinic crystal systems. We have applied

383   the Berreman 4x4 matrix method to derive the MIR optical constants of 5 different pyroxenes for

384   which oriented single-crystal data were not previously reported in the literature. Four spectra with a

385   polarized incident beam at different orientations were acquired for each sample, resulting in three sets

386   of optical constants that can be used to estimate n and k for a randomly oriented powdered sample.

387   These data are necessary to improve compositional estimates of planetary regolith based on radiative

388   transfer models.

389   The data presented here, in conjunction with a coupled optical-thermal model, such as that of

390   Milan et al. (2011), can be used to model MIR emissivity spectra in a vacuum environment relevant to

391   airless solar system bodies. Modeled emission spectra can be compared to emissivity of the lunar

392   surface derived from Diviner Lunar Radiometer data. These optical constants are also applicable to

393   any MIR data from Mars or any airless solar system objects including: existing spectra of asteroids

394   from ISO, Spitzer and any future data from James Webb Space Telescope (JWST) or the OSIRIS-REx

395   mission. Future work will include expanding the current version of the code to include the triclinic

396   case. This code for triclinic minerals will be applied to obtain feldspar optical constants. The Matlab

397   scripts developed for this work will be made publicly available to other researchers at

398   http://aram.ess.sunysb.edu/tglotch/

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688   **Figure and Table Captions**

690   Figure 1. Ternary of pyroxene compositions included in this study.

692   Figure 2. Changes in modeled optical constants (n, k) of orthoclase with initial estimates of ν_j shifted by
693   30 cm^{-1}.

695   Figure 3. Changes in modeled optical constants (n, k) of orthoclase with initial estimates of γ_j shifted by
696   ±50%.

698   Figure 4. Changes in modeled optical constants (n, k) of orthoclase with initial estimates of s_j shifted by
699   ±50%.

701   Figure 5. Changes in modeled optical constants (n, k) of orthoclase with initial estimates of φ_j shifted
702   by ±50%.

704   Figure 6. Changes in modeled optical constants (n, k) of orthoclase with initial estimates of ν_j shifted by
705   30 cm^{-1} and ν_j, γ_j s_j and φ_j shifted by ±50% (top).

707   Figure 7. Measured and modeled reflectance spectra of augite (Aug1) with incident E-field polarization
708   parallel to *a-c* plane at different polarization angles ϕ (top three) and parallel to b (bottom).
709

710   Figure 8. Optical constants (*n*, *k*) of augite (Aug1). In this figure, n1, n2 and k1, k2 are the optical
711   constants for the rays whose polarization direction is parallel to the *a-c* plane, while nb and kb are the optical
712   constants for the rays with polarization direction along the b crystallographic axis.

713

714   Figure 9. Measured and modeled reflectance spectra of augite (Aug2) with incident E-field polarization
715   parallel to *a-c* plane at different polarization angles ϕ (top three) and parallel to b (bottom).

716

717   Figure 10. Optical constants (*n*, *k*) of augite (Aug2). In this figure, n1, n2 and k1, k2 are the optical
718   constants for the rays whose polarization direction is parallel to the *a-c* plane, while nb and kb are the optical
719   constants for the rays with polarization direction along the b crystallographic axis.

720

721   .

722   Figure 11. Measured and modeled reflectance spectra of diopside (Diop1) with incident E-field
723   polarization parallel to *a-c* plane at different polarization angles ϕ (top three) and parallel to b (bottom).

724

725   Figure 12. Optical constants (*n*, *k*) of diopside (Diop1). In this figure, n1, n2 and k1, k2 are the optical
726   constants for the rays whose polarization direction is parallel to the *a-c* plane, while nb and kb are the optical
727   constants for the rays with polarization direction along the b crystallographic axis.

728

729

730   Figure 13. Measured and modeled reflectance spectra of hedenbergite (Hed1) with incident E-field
731   polarization parallel to *a-c* plane at different polarization angles ϕ (top three) and parallel to b (bottom).

732

733   Figure 14. Optical constants (*n*, *k*) of hedenbergite (Hed1). In this figure, n1, n2 and k1, k2 are the optical
734   constants for the rays whose polarization direction is parallel to the *a-c* plane, while nb and kb are the optical
735   constants for the rays with polarization direction along the b crystallographic axis.

736

737

738   Figure 15. Measured and modeled reflectance spectra of orthoclase (Orth1) with incident E-field
739   polarization parallel to *a-c* plane at different polarization angles ϕ (top three) and parallel to b (bottom).

740

741   Figure 16. Optical constants (*n*, *k*) of orthoclase (Orth1) calculated in this work are in the solid lines
742   (n1,k1,n2,k2,nb,kb), while the optical constants derived in Aronson et al. (1986) are in the dashed lines
743   (na1,ka1,na2,ka2,nab,kab).

744

745   Figure 17. Orientation−averaged optical constants in the MIR for several minerals that belong to
746   various crystal systems. Nano-diamonds from a Murchison meteorite (cubic), quartz (hexagonal),
747   olivine (orthorhombic), and diopside (monoclinic).

748

749   Figure 18. Orientation−averaged optical constants (*n*,*k*) of high−Mg olivine ($Mg_{1.9}Fe_{0.1}SiO_4$) from UV
750   to FIR wavelengths (Zeidler et al. 2011). Reflectance spectrum calculated from *n*, *k* values. Labels:
751   Christiansen feature (CF), Reststrahlen bands (RB), highlighted in grey.

752

753   Figure 19. A comparison of single−crystal (enstatite and diopside) vs. amorphous (enstatite and a glass
754   of pyroxene composition) pyroxene optical constants.

755

756   Table 1. Information for pyroxenes and orthoclase included in this study.

757

758   Table 2. Oscillator parameters for Augite (Aug1). The parameters ν, γ, s, ϕ and θ are those described in
759   section 5.1. The standard error, σ, is given for each parameter.

760

761   Table 3. Oscillator parameters for Augite (Aug 2). The parameters ν, γ, s, ϕ and θ are those described
762   in section 5.1. The standard error, σ, is given for each parameter.

763

764   Table 4. Oscillator parameters for Diopside (Diop 1). The parameters ν, γ, s, ϕ and θ are those
765   described in section 5.1. The standard error, σ, is given for each parameter.

766

767   Table 5. Oscillator parameters for Hedenbergite (Hed 1). The parameters ν, γ, s, ϕ and θ are those
768   described in section 5.1. The standard error, σ, is given for each parameter.

769

770   Table 6. Oscillator parameters for Orthoclase (Orth 1). The parameters ν, γ, s, ϕ and θ are those
771   described in section 5.1. The standard error, σ, is given for each parameter.

772

773   **Tables**

774   Table 1.

775

Sample	Source (location)	Chemical formula
augite(Aug1)	SBU (Indian Well, AZ)	$Na_{0.11}K_{0.10}Mg_{0.54}Fe_{0.46}Ti_{0.13}Ca_{0.46}Al_{0.48}Si_{1.79}O_6$
diopside(Diop1)	Kelly's Rocks (Magog, QC)	$Na_{0.04}Mg_{0.64}Fe_{0.18}Mn_{0.01}Ca_{0.92}Al_{0.03}Si_{2.09}O_6$
clinopyx(Aug2)	SBU	$Na_{0.02}Mg_{0.57}Fe_{0.40}Ti_{0.02}Ca_{0.69}Al_{0.13}Si_{2.06}O_6$
hedenbergite(Hed1)	SBU	$Na_{0.03}Mg_{0.29}Fe_{0.51}Mn_{0.07}Ca_{0.83}Al_{0.08}Si_{2.08}O_6$
orthoclase	GGGems (Itrongay, Madagascar)	$K_{0.96}Na_{0.04}Al_{0.96}Fe_{0.04}Si_3O_8$

776

777   Table 2.

j	ν_j	$\sigma(\nu_j)$	γ_j	$\sigma(\gamma_j)$	s_j	$\sigma(s_j)$	φ_j	$\sigma(\varphi_j)$	θ_j
1	1106.3575	0.4039	13.6440	1.4160	4710.7187	519.6075	33.7390	2.2315	90
2	1082.0787	0.7336	22.4311	2.8987	8993.4843	1526.8844	57.9436	2.2866	90
3	1049.0371	0.1930	34.2430	0.6058	179324.6400	2855.2145	71.6003	0.2040	90
4	1010.1750	0.5134	20.6827	1.4914	15743.7790	1164.9098	33.9720	1.4204	90
5	973.9422	1.2439	39.3002	2.5816	61647.1074	7198.6643	100.6033	1.9936	90
6	952.8605	0.6238	33.8723	1.1586	115080.9250	3657.2602	76.5908	1.6294	90

7	911.9700	1.9049	60.9354	5.4555	84647.1159	6815.1152	69.0827	1.9607	90
8	944.8770	0.6580	48.8271	2.4135	96156.4057	6739.0871	130.0419	2.5202	90
9	864.4122	0.4977	43.8169	1.0250	236251.8770	364.8184	1.5422	0.5618	90
10	855.2310	0.9153	31.8268	2.0963	73587.6460	1012.5941	148.5916	2.1071	90
11	768.1230	1.8893	89.4754	7.2442	55510.9508	4229.1492	106.3017	2.6079	90
12	628.8353	0.2212	18.0435	0.7495	33689.7859	1649.9417	101.0689	0.8103	90
13	558.8928	0.5426	20.5635	1.7036	3907.3075	383.2433	-1.2976	4.3107	90
14	527.2604	0.5724	24.0277	2.0407	10163.0101	1027.2230	2.9381	3.4734	90
15	511.0346	0.6194	42.7838	2.2268	48307.6346	3153.4361	113.9736	1.4942	90
16	588.4716	5.8446	86.0548	18.4170	24961.4935	5574.7554	89.6034	3.3377	90
17	487.9342	0.3804	27.1740	1.2809	59799.8695	3570.4805	-7.2227	0.8682	90
18	452.2373	0.2418	29.8619	0.7627	256324.4190	4869.1466	-7.2227	0.1871	90
19	378.5617	0.2780	36.6437	1.4695	53084.6470	8107.2438	84.8518	6.4041	90
20	380.5842	1.0044	53.7977	4.0509	72332.4613	6006.1467	25.3526	6.0986	90
21	316.6041	0.1706	22.8939	0.3635	121807.2190	1236.6558	76.0592	0.3385	90
22	285.8952	0.3018	26.1164	0.7252	78823.7304	1650.5374	141.5585	0.5527	90
23	1066.2639	0.1892	30.6764	0.2559	222090.2320	1434.7913	0	--	0
24	963.3500	0.2452	24.6545	0.6687	89492.5772	2397.4128	0	--	0
25	900.8600	0.5216	61.1955	1.6569	210326.1180	4518.3363	0	--	0
26	673.6817	1.2406	34.7883	3.7145	19978.7527	1653.7995	0	--	0
27	547.9000	0.4589	18.9619	1.7624	6433.4126	786.4962	0	--	0
28	503.9100	0.2723	37.6983	0.8500	148239.2660	4230.4820	0	--	0
29	473.3900	0.2018	18.3338	0.6366	104023.2710	2914.9693	0	--	0
30	408.0200	0.4402	21.1392	1.4232	26911.5056	1472.1208	0	--	0
31	367.1695	1.0108	22.6618	4.1379	12240.3510	2468.8277	0	--	0
32	333.8303	0.7396	37.0955	2.4841	44673.8703	2939.0821	0	--	0

| ε_{xx}=2.3418(0.0040) | | ε_{xy}=0.0263(0.0036) | | ε_{yy}=2.3934(0.0030) | | | ε_{zz}= 2.6441(0.0043) | | |

778

779   Table 3.

j	ν_i	$\sigma(\nu_i)$	γ_i	$\sigma(\gamma_i)$	s_i	$\sigma(s_i)$	φ_i	$\sigma(\varphi_i)$	θ_i
1	1061.3863	1.6775	16.7945	3.5355	24107.2736	9108.7181	109.9541	3.0586	90
2	1045.6266	1.0695	17.4601	4.5891	49146.8143	15451.7954	118.8724	1.4748	90
3	1021.4581	1.8514	25.7043	6.2705	46430.9850	12385.4430	125.3247	2.1043	90
4	992.3639	1.1743	36.2713	3.4181	26819.2312	2845.9399	4.0808	7.8728	90
5	950.6749	1.8544	56.3535	3.6006	350600.2530	198.6376	92.4733	1.0478	90
6	873.6918	3.5412	73.3247	7.0740	198501.9250	4841.0644	103.9087	5.7859	90
7	852.6279	0.9302	56.1304	2.4576	384449.5580	21164.2827	-0.0526	2.7969	90
8	768.7863	3.5090	100.1498	11.8050	351227.4630	80.4223	-35.0603	1.7465	90
9	600.0011	3.0444	103.2869	9.5882	345195.2700	27533.1404	-49.3688	1.6754	90
10	686.4430	3.5464	112.2921	13.4456	157635.0660	22704.7234	15.7006	3.6531	90
11	625.9819	1.2538	25.3481	4.3195	31759.5593	5445.8591	73.3052	5.5194	90
12	520.0000	1.4388	20.2592	3.8818	55527.2990	8895.0274	82.9539	8.5934	90
13	533.0903	2.2436	17.2663	6.5846	26237.0233	1283.3818	179.8287	8.5146	90
14	501.7328	1.5229	22.9771	4.8641	168521.7630	27.0692	8.2681	4.3965	90
15	479.9509	0.7686	16.6904	2.6651	294597.8250	25.7761	4.6831	2.0602	90
16	461.8681	0.8220	14.9005	1.5448	258672.0850	1733.0123	5.0887	1.8157	90
17	403.8875	1.6247	34.3784	4.1294	86703.4089	6799.8357	99.5010	4.3104	90
18	360.1886	6.2701	27.2829	19.1020	17351.0619	11466.8151	-7.5571	14.6287	90
19	332.0028	1.0169	21.7865	3.0345	38951.2369	4767.2072	72.8595	5.0749	90
20	281.8601	1.4334	41.1500	3.7859	226289.1590	41.8564	32.8478	1.1554	90
21	250.0777	4.5801	15.2753	5.7124	41555.6458	23085.6849	74.3621	10.3421	90
22	1077.2920	0.4198	22.8731	0.6367	149503.0950	2402.3553	0	--	0
23	964.0978	1.2006	48.8749	4.5997	138155.7890	15182.2000	0	--	0
24	899.9383	3.5474	106.4168	7.3552	286332.2180	24390.6181	0	--	0

25	684.1713	5.8182	108.5547	25.4532	66276.4418	26720.9365	0	--	0
26	557.1254	1047.5670	15.2229	666.7554	3104.1971	177321.3230	0	--	0
27	541.0487	3.4361	17.7469	31.3527	9273.8041	161727.1810	0	--	0
28	524.2434	1.6431	18.0151	10.7360	19617.9937	16815.8158	0	--	0
29	507.6945	0.5276	18.0932	2.3374	67758.0486	12997.2329	0	--	0
30	480.6085	0.8391	31.0358	2.9332	173741.2560	16787.0322	0	--	0
31	411.3853	5.8307	45.1586	20.6277	61591.7484	47708.6593	0	--	0
32	370.1525	19.3001	44.4246	135.0416	23586.7622	91495.5373	0	--	0
33	325.5302	12.2621	65.4127	22.8392	72943.9747	51540.5930	0	--	0
34	257.0514	0.9801	12.4295	2.7168	16853.4601	3824.3130	0	--	0
$\varepsilon_{xx}=3.1888(0.0147)$		$\varepsilon_{xy}=0.0050(0.0168)$			$\varepsilon_{yy}=2.8116 (0.0157)$			$\varepsilon_{zz}= 2.6090 (0.0109)$	

780

781   Table 4.

j	ν_i	$\sigma(\nu_i)$	γ_i	$\sigma(\gamma_i)$	s_i	$\sigma(s_i)$	φ_i	$\sigma(\varphi_i)$	θ_i
1	1053.3492	0.2690	9.8041	0.5202	161807.4260	8449.4644	95.0619	0.5386	90
2	1038.6875	0.4434	11.9789	1.1319	102002.5840	8297.6460	81.8839	0.7175	90
3	987.1730	1.1344	22.0697	2.3375	43276.2855	8424.1418	-58.3177	1.7571	90
4	961.9418	0.5321	21.8740	1.4044	328246.2610	13426.1056	107.2574	0.4212	90
5	908.9778	1.2771	34.1717	3.7573	112024.9180	10847.7536	88.2555	1.2813	90
6	851.9349	0.7393	52.0897	1.8660	276075.0410	8603.7134	40.6706	1.1639	90
7	799.5717	2.9359	82.3099	8.5987	133499.1160	11910.3499	140.7057	2.6738	90
8	694.3785	2.9357	139.0056	9.4790	184063.9650	11455.4558	35.9865	1.6679	90
9	625.9676	0.6184	20.9614	1.1518	85562.6394	3066.4869	111.9229	0.8129	90
10	526.8297	1.7909	48.7469	3.7816	97271.7196	11572.2554	45.1962	1.4457	90
11	509.9354	0.7947	14.1122	2.1296	16820.8129	2318.7730	-38.9575	4.1582	90
12	488.7702	1.0874	25.2207	3.2101	102617.7860	14753.3418	51.9415	1.9863	90
13	462.0420	0.8680	37.2480	2.3266	302939.5670	16231.8191	21.2456	0.8955	90

14	379.4407	0.6114	32.5722	1.2839	117538.4980	4685.8259	112.1053	0.9140	90
15	326.4878	0.9753	26.4854	2.6635	108243.6900	14930.1059	-66.8801	1.1360	90
16	297.4023	1.4361	27.9642	5.2131	98661.8029	17147.5147	-59.4064	4.2180	90
17	293.0303	0.7230	16.9140	1.9692	26130.5743	3123.2116	20.9335	12.1318	90
18	236.8182	2.6280	14.3421	3.0202	49054.5289	8115.4718	10.1390	6.1075	90
19	1065.2649	61.4940	50.5334	1.8536	136867.0000	139.1562	0	--	0
20	954.2127	50.9689	35.3480	3.5371	65646.0001	54.6979	0	--	0
21	913.3331	114.3238	31.7870	6.9236	42070.0001	24.6549	0	--	0
22	863.7441	367.8407	126.8820	24.7606	195784.2720	54551.0765	0	--	0
23	737.9597	2678.3443	140.9497	56.2231	92809.1745	52723.1287	0	--	0
24	636.0029	552.8693	93.0399	9.7740	89888.9079	17968.0509	0	--	0
25	504.2384	645.0038	31.7429	1.4460	163435.8470	13745.7938	0	--	0
26	472.0973	792.9559	28.4750	1.9606	276342.9090	15861.7259	0	--	0
27	413.8197	324.9801	26.0624	3.2501	70136.7282	7278.4287	0	--	0
28	249.2397	277.7731	9.7763	1.2649	18139.7810	2824.9225	0	--	0
ε_{xx}=2.2120(0.0092)		ε_{xy}=0.0084(0.0109)			ε_{yy}=3.2076(0.0107)			ε_{zz}= 2.3310(0.0111)	

782

783

784

785   Table 5.

j	ν_i	$\sigma(\nu_i)$	γ_i	$\sigma(\gamma_i)$	s_i	$\sigma(s_i)$	φ_i	$\sigma(\varphi_i)$	θ_i
1	1085.5086	1.0619	53.6032	2.0797	71057.9148	10.0624	77.0368	1.6560	90
2	1059.2960	0.5518	45.6650	1.1514	159377.0460	3792.4402	-48.5292	0.5769	90
3	993.1131	1.1689	26.9090	3.5555	9922.7969	2381.2746	38.0265	7.7690	90
4	967.4469	0.8350	45.8181	2.5602	95361.6473	4969.2601	84.6362	1.1185	90
5	904.4503	1.5764	39.7557	4.0140	17736.2350	2895.3918	9.7179	4.8795	90
6	854.4819	0.3215	34.8501	0.7845	359324.3050	3685.3273	8.2315	0.2746	90

7	627.1273	0.4077	18.5918	0.9474	22454.7292	809.0312	70.7968	1.0661	90
8	554.0051	0.8223	20.0375	2.2529	11125.4731	935.6338	80.3744	1.5719	90
9	498.4405	0.5100	36.7979	1.1952	47045.1989	1737.4115	31.5953	0.6441	90
10	444.5136	0.2360	25.4438	0.5064	259681.5030	2531.5769	7.0115	0.1641	90
11	365.7561	0.4065	40.0052	1.1436	115793.2740	2579.3708	-17.1310	0.3263	90
12	316.5364	0.2868	17.5481	0.7074	79478.0308	2327.4479	146.8989	0.4168	90
13	295.8607	0.2829	11.2035	0.8214	38037.8982	2341.3446	-10.7030	0.9746	90
14	269.8787	0.2434	11.4372	0.5673	24979.2863	1003.2629	31.7790	0.9470	90
15	1058.5000	0.1466	13.5591	0.1493	298081.4700	1586.6960	0	--	0
16	954.2000	0.1756	15.9576	0.3435	155456.8690	2858.5771	0	--	0
17	905.3000	0.3818	37.5829	1.0258	283403.9260	5357.2963	0	--	0
18	661.1000	1.2062	61.1123	3.4700	68518.4267	3042.9618	0	--	0
19	509.4000	0.2300	25.7632	0.3148	236134.3190	3062.6966	0	--	0
20	471.8000	0.2540	14.0770	0.6940	81073.6183	2729.1871	0	--	0
21	398.1000	0.3743	23.0772	1.0692	64178.4958	2420.5236	0	--	0
22	363.7127	0.6361	14.3740	2.4526	17497.1025	3048.7496	0	--	0
23	330.9739	1.4859	43.8902	5.1669	49615.4221	5331.1122	0	--	0
24	277.0999	0.3965	9.3079	1.2061	11291.1774	1162.9514	0	--	0
ε_{xx}=2.323433(0.005738)		ε_{xy}=0.011083(0.004933)			ε_{yy}=1.811383(0.004054)		ε_{zz}= 3.476333(0.0063)		

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787   Table 6.

j	ν_j	$\sigma(\nu_j)$	γ_j	$\sigma(\gamma_j)$	s_j	$\sigma(s_j)$	φ_j	$\sigma(\varphi_j)$	θ_j
1	1128.3686	0.3431	31.2995	0.7423	54556.3167	2123.2030	144.4339	1.2192	90
2	1108.8571	0.5588	31.1108	0.5308	212226.6890	3795.8550	24.3628	0.4137	90
3	1027.3708	0.3793	33.1247	0.6044	363554.0780	18.0570	96.9297	1.5021	90
4	1037.7416	0.5378	30.7390	1.3144	141912.7300	17.9877	4.6421	2.7087	90
5	1009.9518	0.4677	22.2564	1.0482	172752.3130	5177.9700	175.9980	1.8392	90

6	991.7254	0.5793	24.2304	2.0259	150428.1450	11517.6300	103.3195	1.8847	90
7	765.4734	3.4041	42.0367	10.9087	15482.5298	3241.5640	5.9023	6.1221	90
8	718.5118	1.2856	27.2765	3.9460	20263.4125	2306.1400	-51.0158	3.5496	90
9	638.1094	0.4900	17.9200	1.1941	28666.8966	1392.3170	145.0234	1.2033	90
10	578.8337	1.6291	24.5589	1.0170	42223.7579	9406.2510	43.3327	1.7890	90
11	570.6447	0.5394	11.6388	0.7779	73786.7114	488.4382	42.3799	1.2196	90
12	563.4729	0.7157	9.2861	1.9959	35232.0422	9229.9400	39.1535	2.2532	90
13	415.7642	0.5353	34.7887	0.7423	114579.3000	1911.6290	-41.7658	0.4592	90
14	1135.3801	0.8506	39.8303	2.1129	14854.1612	1579.1328	0	--	0
15	1102.8937	0.5060	42.5629	2.0172	32799.5356	2104.3277	0	--	0
16	1020.6898	0.5366	42.7108	0.7767	259002.7780	13008.0113	0	--	0
17	992.4225	0.2744	32.1287	0.8942	387229.1360	12639.2520	0	--	0
28	774.4806	1.3876	22.3337	4.0335	15639.1124	4074.5787	0	--	0
19	752.3726	1.4388	23.5478	7.5651	15823.7692	6397.6618	0	--	0
20	725.7595	1.3542	25.5395	3.9808	18424.9031	3558.0395	0	--	0
21	610.5486	0.5855	17.5118	1.7004	11599.0969	836.4948	0	--	0
22	543.0700	0.2560	16.9498	0.6631	31705.6149	1032.8273	0	--	0
ε_{xx}=2.0658(0.0111)		ε_{xy}=0.0043(0.0085)			ε_{yy}=2.0126(0.0107)			ε_{zz}=2.4461(0.0033)	

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Hedenbergite(Hed1)