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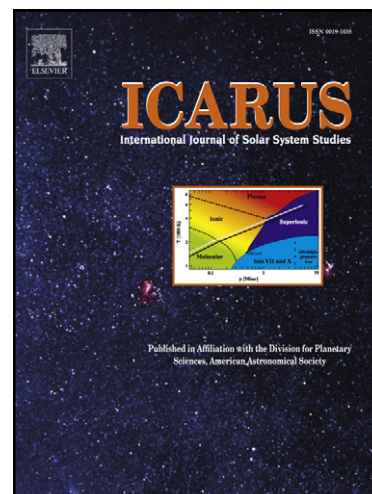
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25 Abstract

26
27 An automatic procedure has been implemented on the original MGM approach (Sunshine et al.,
28 1990) in order to deal with an a priori unknown mafic mineralogy observed in the visible-near infrared by
29 reflectance spectroscopy in the case of laboratory or natural rock spectra. We consider all the mixture
30 possibilities involving orthopyroxene, clinopyroxene and olivine, and use accordingly for each
31 configuration different numbers of Gaussians, depending on the potential complexity of the mixture. A
32 key issue is to initialize the MGM procedure with a proper setting for the Gaussians parameters. An
33 automatic analysis of the shape of the spectrum is first performed. The continuum is handled with a
34 second order polynomial adjusted on the local maxima along the spectrum and Gaussians parameters
35 initial settings are made on the basis of laboratory results available in the literature in the case of simple
36 mixtures of mafic minerals. The returned MGM solutions are then assessed on spectroscopic grounds and
37 either validated or discarded, on the basis of a mineralogical sorting.

38 The results presented in this paper are a first quantitative step to characterize both modal and
39 chemical compositions of pyroxenes and olivines. A demonstration of the methodology on specific
40 examples of binary and ternary olivine-pyroxenes mixtures has been made, which shows that the different
41 non-linear effects which affect the Gaussian parameters (center and strength) can be successfully handled.
42 Of note is the fact that the band center positions associated with the different mafic minerals are not set
43 here in the inverse problem, and thus the MGM outputs are truly informative of the chemical composition
44 of pyroxenes and olivines. With the consideration of some limits on the detection thresholds, these results
45 are quite promising for increasing the operational use of the Modified Gaussian Model with large
46 hyperspectral data sets in view of establishing detailed mineralogical mappings of magmatic units.

47

48 Keywords: Reflectance spectroscopy, Mineralogy, Spectral deconvolution, MGM

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52

53 1. Background

54 In the field of reflectance spectroscopy, determination and characterization of mafic mineralogies
55 have been a major area of investigation for the last 30 years (e.g., Adams, 1974; Mc Cord et al., 1981;
56 Singer, 1981; Cloutis and Gaffey, 1991; Bishop et al., 1998; Harloff and Arnold, 2001; Schade et al.,
57 2004; Pompilio et al., 2007). A progressive amount of complexity has been introduced in the description
58 of spectra with the aim of extracting the relevant spectral information (e.g., albedo, slope of the
59 continuum, position and depth of the absorption bands...) for mineralogy purposes.

60 Though its physical meaning is not thoroughly understood, the continuum plays an important role
61 in all spectral analyses and particularly in MGM deconvolution (e.g., Clark and Roush, 1984; Harloff and
62 Arnold, 2001; Clark et al., 2003). It is of particular relevance to define a continuum close to the spectrum
63 global shape in order to best isolate the absorbing features at all wavelength.

64

65 1.1 Olivine and pyroxene spectroscopy

66

67 In visible and near-infrared reflectance spectra, olivine and pyroxenes are characterized by their
68 Fe²⁺ electronic transition absorption bands. For a perfect octahedral crystal field, the electronic transition
69 creates an absorption feature with a minimum around 1.10 μm . However, absorptions of a same metallic
70 ion can occur at different wavelengths because of variations in the crystallographic site symmetry, bond
71 type and length and site distortion (Burns, 1993) and absorption width is linked to thermal vibrations that
72 modify the bond length around a mean value (Burns, 1993).

73 Consequently, pyroxenes reflectance spectra show two main absorptions respectively around 1
74 and 2 μm and a less pronounced absorption at 1.2 μm (Hunt and Salisbury, 1970; Adams, 1974, 1975;
75 Singer, 1981; Klima et al., 2007). This 1.2 μm absorption is the result of molecular distortion in the M₁

76 crystallographic site (Burns, 1993). Nevertheless, clinopyroxene spectra are much more variable than
77 orthopyroxene spectra and two main spectral types have been identified (Adams, 1975). Absorptions of
78 spectral type B, much more common in most geological settings, correspond to those described above.
79 Spectral type A clinopyroxene, where there are major contributions from ferrous iron in the M_1 site will
80 results in absorption band near 0.9 and 1.15 μm and no band at 2 μm (Adams, 1975; Cloutis and Gaffey,
81 1991). Spectra of olivine are dominated by a broad complex absorption feature which is a composite of
82 several absorptions: two of them correspond to iron in the M_1 site (around 0.85 and 1.25 μm) while the
83 third one, around 1.05 μm , corresponds to the M_2 site (Burns, 1970; Hunt, 1977).

84 The substitution of different sized cations, such as calcium, iron and magnesium, also controls the
85 positions of the different absorptions minima. In the case of olivine $[(\text{Mg,Fe})_2\text{SiO}_4]$, solid-solution ranges
86 from forsterite to fayalite. The overall position of the 1.0 μm absorption feature is known to shift toward
87 longer wavelengths with increasing iron content (Burns, 1970, 1993; Adams, 1975; King and Ridley,
88 1987). For pyroxenes $[(\text{Ca,Mg,Fe})_2\text{Si}_2\text{O}_6]$, wavelengths shift is function of $\text{Fe}/(\text{Mg}+\text{Fe}+\text{Ca})$ ratio (Adams,
89 1974, 1975; Cloutis et al., 1986; Cloutis et Gaffey, 1991). Basically, enstatite (orthopyroxene) main
90 absorptions occur around 0.90 and 1.85 μm , while diopside (clinopyroxene) main absorptions occur
91 around 1.00 and 2.30 μm (Hunt and Salisbury, 1970; Adams, 1974, 1975; Singer, 1981). The difference
92 between the two types of pyroxenes is related to Fe^{2+} position: metallic ion is located preferentially in M_2
93 site for orthopyroxene and in M_1 site for clinopyroxene, Ca^{2+} being in M_2 site in the second case (Adams,
94 1974; Burns, 1993). In the case of orthopyroxene endmember (enstatite-ferrosilite), as there is almost no
95 calcium in the structure, the wavelength shift is directly function of the $\text{Fe}/(\text{Mg}+\text{Fe})$ ratio. Hazen et al.
96 (1978), followed by Cloutis and Gaffey (1991), have shown that absorption features evolve progressively
97 between the pyroxenes endmember, absorption minima shifting to longer wavelength with increasing Fe
98 content (diopside to hedenbergite and enstatite to ferrosilite) and Ca content (enstatite - pigeonite - augite
99 - diopside).

100 On these grounds, the retrieval of characteristics of mafic minerals from unknown reflectance
101 spectra does not appear as an impossible task and would be indeed of great use for the remote
102 mineralogical analysis of planetary surfaces. However, today the direct interpretation of a spectrum is still
103 limited as it is hampered by the overlap of the absorption features, particularly when there is a mixture of
104 two or three minerals, as it is frequently the case with rocks. Indeed, such spectra show intermediate
105 properties to the different endmember components. Those properties vary non-linearly as a function of
106 minerals relative abundance and composition (Adams, 1974; Singer, 1981; Cloutis and Gaffey, 1991) and
107 the key issue is to be able to deconvolve unambiguously a complex spectral shape measured either on a
108 laboratory sample or from orbit, in order to detect and characterize the different endmember components.
109 The Modified Gaussian Model (MGM), developed by Sunshine et al. (1990), has the potential to resolve
110 the endmember contributions.

111

112 1.2 Use of the Modified Gaussian Model (MGM) for mafic mineral assemblages

113

114 The principle of the Modified Gaussian Model is to deconvolve overlapping absorptions of mafic
115 mineral spectra into their fundamental absorption components. The specific interest of this model is to
116 directly account for electronic transition processes (e.g., Sunshine et al., 1990). Consequently, the MGM
117 approach is in essence able to achieve a direct detection and quantification of minerals which make up the
118 observed surface.

119 The pioneering work by Sunshine et al. (1990) relies on the fact that spectrum variations in visible
120 and near-infrared are caused by absorption features that can be described by means of Gaussians (Clark
121 and Roush, 1984). Sunshine et al. (1990) used modified Gaussians to obtain a mathematical solution
122 closer to the physical reality. Each Gaussian is parameterized by a band center, band width and band
123 strength. As described in Sunshine and Pieters (1993), MGM computations are carried out in energy and
124 natural log reflectance space. Thereby, overlapping absorptions are additive and can be modeled using
125 linear inverse theory. The method applied is the stochastic inversion of Tarantola and Valette (1982) that
126 permits the introduction of a priori information as constraints on the solutions. These constraints are
127 defined by means of uncertainties, applied on each starting parameter and set as a function of considered
128 absorptions. During the non-linear least-squares iterative process, Gaussians and continuum parameters
129 vary until the residual errors are minimized (Sunshine et al., 1990; Sunshine and Pieters, 1993). The
130 residual errors are calculated as the difference between the log of the actual spectrum and the log of the
131 modeled spectrum. Spectra are modeled in the logarithm of reflectance space as a sum of modified
132 Gaussian distributions superimposed on a baseline continuum. The resulting combinations of Gaussians
133 can then be interpreted in terms of mineralogy.

134 Sunshine and Pieters (1993, 1998) first results dealt with cases involving simple mafic
135 mineralogies, i.e. either olivine alone or pyroxenes only mixtures. This work will be used as a reference in
136 our following study. Using three Gaussians in their model, Sunshine and Pieters (1998) have been able to
137 characterize systematic trends linked to M_1 and M_2 sites for olivine, with a progressive increase with
138 higher iron content of both band center positions toward longer wavelength and of the 1.05 μm band
139 intensity relative to the 1.2 μm feature. Widths did not show any special trend.

140 Sunshine and Pieters (1993) also studied mixtures of two pyroxenes with fixed chemical
141 compositions and succeeded in deconvolving the suite of spectra in terms of endmember absorptions.
142 They showed that while the center and width of the absorption bands did not depend on the mineral
143 proportions, the relative abundances of the two pyroxene minerals could be directly linked to the
144 Gaussians strength.

145 At first order, in the case of simple mineralogies, MGM is thus able to retrieve modal and/or
146 chemical composition from an unknown spectrum. Successive studies have shown the interest of the
147 MGM approach for planetary surface characterization (e.g., Mustard and Sunshine, 1995; Mustard et al.,
148 1997; Noble et al., 2006; Kanner et al., 2007). However, one should note that for the reference studies, all
149 the spectra used were acquired on controlled laboratory powder samples, with grain size between 24 and
150 250 μm . Kanner et al. (2007) have also pointed out that the MGM returned solutions were sensitive to
151 some extent to the band centers initialization.

152 So far, more complex situations addressing complex mineralogies (i.e. olivine and pyroxene(s)
153 and/or different pyroxene composition) and/or rock samples (e.g., Pompilio et al., 2007) have been little
154 explored by the MGM approach at the exception of a few recent works (e.g., Pompilio et al., 2006;
155 Pompilio et al., 2009; Parente and Bishop, 2006; Pinet et al., 2006, 2007, 2009; Clenet et al., 2008, 2009)
156 and significant efforts have to be made in this direction for improving our capability of spectroscopic
157 modeling and interpretation when dealing with real world observations of unknown mafic rock lithologies
158 observed under natural conditions. Our goal here is to improve the capability of the MGM to realistically
159 model complicated mafic mineralogies.

160

161 1.3 Laboratory data sets

162

163 Our present study relies on laboratory data of synthetic mixtures with different grain sizes and
164 natural rocks, mainly taken in the Reflectance Experiment Laboratory (RELAB) database at Brown
165 University. Measurements have been produced using a bidirectional near-infrared spectrometer ($i=30^\circ$
166 and $e=0^\circ$) from 0.5 to 2.5 μm (Pieters, 1983; Pieters and Hiroi, 2004).

167 Spectra include olivine ranging from forsterite to fayalite (including some of the data used by
168 Sunshine et al. (1998)), different types of pyroxene alone and mixtures (including the ones from Sunshine
169 et al. (1993) and part of Klima et al. (2007)). We also use olivine and orthopyroxene mixtures (Mustard
170 and Pieters, 1989; Hiroi and Pieters, 1994).

171

172 2. Methodology

173

174 2.1 Initialization driven by mineral chemical composition with application to mineralogical mixtures

175

176 The Modified Gaussian Model code we use in this paper is the one described by Sunshine et al.
177 (1990, 1999). It can be downloaded at <http://www.planetary.brown.edu/mgm/>. However, modifications
178 about the continuum and the Gaussians characteristics, as well as an automation of the procedure, have
179 been introduced. Specificities of our approach are described hereafter.

180 MGM directly takes into account electronic transition processes; consequently, the number of
181 Gaussians which should be used for a given deconvolution directly depends on the number of absorption
182 bands present in a spectrum. As described above, three Gaussians are needed to characterize either an
183 olivine or a pyroxene. Each absorption feature has a center which may vary in a specific range as a
184 function of the mineral chemical composition (Adams, 1974; Hazen et al., 1978; Cloutis and Gaffey,
185 1991; Sunshine and Pieters, 1998). In this paper, Gaussians will be named accordingly to their respective
186 band center initialization (e.g. the Gaussian which models clinopyroxene absorption between 980 and
187 1050 nm will be named Gaussian "1000"). So, olivine absorptions will be modeled by Gaussians "850"
188 (ranging between 840-900 nm), "1050" (1040-1075 nm) and "1250" (1200-1300 nm); spectral type B
189 clinopyroxene absorptions by Gaussians "1000" (980-1050 nm), "1200" and "2150" (2050-2350 nm);

190 orthopyroxene absorptions by Gaussians “900” (895-970 nm), “1200” and “1800” (1800-2100 nm). In
191 our approach, we do not consider spectral type A clinopyroxenes and “clinopyroxene” will further refer to
192 spectral type B clinopyroxene.

193 Two additional Gaussians are also required to obtain physically realistic modeling. The first one,
194 centered around 450 nm, is used to model the strong large absorption at shorter wavelength (i.e. charge
195 transfer in ultraviolet). The second one, centered around 650 nm, may account for a small pyroxene
196 absorption, especially in the case of composition close to diopside (Sunshine and Pieters, 1993; Klima et
197 al., 2007). This absorption may be attributable to ferrous-ferric iron charge transfer (Cloutis, 2002). Both
198 Gaussians also contribute stabilizing the overall shape of the continuum in the visible domain.

199 In the case of an unknown mafic rock, the strategy is to consider that all the combinations between
200 the three different minerals are possible. A set of Gaussians, dedicated to a specific mineralogy, will be
201 called further “configuration” (e.g. olivine configuration, orthopyroxene configuration, orthopyroxene-
202 clinopyroxene configuration...). In our problem, the number of configurations amounts to seven. In the
203 case of the simplest configurations, four or five Gaussians are required to model a spectrum (cf. Tab. 1).
204 Additional Gaussians are added in the case of mixtures. However, identical Gaussians which appear for
205 two or more minerals are used only once (i.e. absorption around 1200 nm for the two pyroxenes (Noble et
206 al., 2006). Moreover, in the case of olivine-pyroxene mixtures, the pyroxene absorption around 1200 nm
207 is masked by the olivine one. In this case, the choice is made for the time being not to use the Gaussian
208 1200 dedicated to pyroxene. Accordingly, nine Gaussians are used in the most complicated case which
209 addresses a ternary mixture. The different combinations used for every configuration are reported in
210 Table 1.

211 Following from what has been explained earlier in section 1.2, each Gaussian has to be initialized
212 with a band center and an uncertainty on this parameter. The uncertainties on the Gaussians parameters
213 have been set in such a way that our MGM modeling may encompass the range of spectral changes
214 associated with chemical compositions of pyroxene and olivine. A number of tests have driven us to fix a
215 band center uncertainty of 200 nm for all the Gaussians in the 1 μ m domain, and 400 nm in the 2 μ m
216 domain.

217

218 2.2 Initialization considering laboratory samples and natural rocks

219

220 2.2.1 Continuum

221

222 For laboratory data, the global shape of a spectrum is usually quite flat. The continuum, as defined
223 by Clark and Roush (1984), was initially taken as a straight line. In the original version of the MGM,
224 Sunshine and Pieters (1993) have chosen a continuum which is linear in energy. This continuum is
225 controlled by two parameters, respectively linked to the slope and to the shift in reflectance. In
226 wavelength space, such a continuum comes as a flat line in infrared and a curved line at shorter
227 wavelengths.

228 In the present study, the undertaken MGM approach is intended to model laboratory spectra as
229 well as natural rock spectra. As illustrated in Figure 1 for the case of diopside, the spectra of different
230 grain-sized powders exhibit obvious differences from bulk rocks of a similar composition measured in the
231 field. The physical rock texture is the major cause for these spectral differences. Laboratory spectra with
232 larger grain size ($>45\mu\text{m}$) look more similar to the natural data than the small grain size spectrum
233 ($<45\mu\text{m}$). The presence of varnish at the surface (e.g. desert varnish) may also contribute to the spectral
234 signature in the case of natural rocks. The observed differences can be generally ascribed to photometric
235 and environmental (e.g. varnish, alteration) or saturation effects (Combe et al., 2006; Pompilio et al.,
236 2007; 2009; Roy et al., 2009). The general characteristics are as follows: i) variations of the reflectance
237 mean level; ii) lower reflectance level at longest wavelength (i.e. around $2.5\mu\text{m}$); and iii) weaker relative
238 strength of the spectral absorptions.

239 By definition, the variations of the reflectance mean level are handled by the continuum in the
240 MGM deconvolution. For the second effect, tests have shown that a straight line continuum will
241 significantly overestimate the infrared absorption(s) strength(s) in the case of natural rocks as the
242 continuum is strongly controlled by the local maxima at $0.6\text{-}0.8\mu\text{m}$ and $1.5\text{-}1.6\mu\text{m}$. The choice of a
243 second order polynomial continuum in wavelength space clearly improves the situation. Such a
244 continuum is defined by three parameters which correspond respectively to the average reflectance level,
245 the global slope and the function curvature. That way, the overall shape of the continuum better describes
246 the general spectral trend of any spectrum all along the visible-near infrared domain and as a result,
247 Gaussians strength will better characterize the real absorption strength.

248 Though its physical meaning is not thoroughly understood, the continuum plays an important role
249 in all spectral analyses and particularly in MGM deconvolution (e.g., Clark and Roush, 1984; Harloff and
250 Arnold, 2001; Clark et al., 2003). It is of particular relevance to define a starting continuum close to the
251 spectrum global shape in order to best isolate the absorbing features at all wavelength. This is achieved
252 from a spectral shape analysis, based on an automatic procedure detecting the local minima and maxima
253 along the spectral domain (cf. Fig. 2). This information will also be quite useful for the initialization of
254 the Gaussians to be used as described in section 2.2.3. The coefficients of the polynomial are set so that
255 the starting continuum is defined as a smooth mathematical function. This function is constrained by the
256 main maxima detected along the spectrum and used as anchor points, though the final continuum (after
257 running the MGM) may not be necessarily tangential to the spectrum, with the advantage that its overall
258 shape is not controlled by a restricted spectral range.

259

260 2.2.2 Influence of initialization on the MGM results

261

262 Consequently to the use of a generalized inversion approach, the MGM results are sensitive to
263 Gaussians centers initializations, and a variation has been found between the MGM calculated absorption
264 center and the real mineralogical absorption center (Kanner et al., 2007). In the case of laboratory data,
265 variation ranges are on the order of ± 8 and ± 17 nm, respectively for the $1\mu\text{m}$ and $2\mu\text{m}$ domain

266 absorptions. As a complement, we assess in the following the influence of Gaussians strength
267 initialization on the MGM results. The sensitivity of the MGM is here tested considering the initial
268 strength of the Gaussians compared to the strength of the mineralogical absorptions. To do that, we make
269 systematic tests considering those parameters. Principle and results are described hereafter.

270 For a given spectrum, we vary the initialization of the Gaussians strength parameter, all the
271 Gaussians of the set having an identical initial strength. At the same time, we consider a series of
272 synthetic spectra showing absorptions strengths ranging from “laboratory” case to “natural” case. To
273 simulate the case of “natural” spectra (cf. Fig.1, i.e. keeping a strictly identical chemical composition but
274 showing weaker absorptions), we choose to use laboratory spectra which are artificially flattened.
275 Reflectance logarithm is thus multiplied by the same factor at all wavelengths. That way, the higher the
276 flattening rate, the flatter the spectrum with a higher reflectance level. Examples of four synthetic spectra
277 are shown in Figure 3-A. The laboratory reference spectrum considered here is a mixture of
278 orthopyroxene and clinopyroxene, with particle size between 45 and 75 μm , taken from the Sunshine and
279 Pieters (1993) set.

280 For all our tests (see graphs on Figures 3-B and 3-C), calculations are made by varying the
281 flattening rate with a 1% step. Initial Gaussians strengths range from -0.3 to 0 by step of 0.05. Final
282 centers and strengths are calculated using the MGM in all the parametric space and visualization is based
283 on a color scale. High band center positions, or large strengths, correspond to red shade; conversely low
284 band center positions, or weak strengths, correspond to blue shade. If initialization has no influence,
285 results should show throughout the parametric space:

286 -i) the same value regarding the center of each Gaussian associated with a given absorption feature, close
287 to the one determined by Sunshine and Pieters (1993) (with a possible variability on the order of that
288 defined by Kanner et al. (2007));

289 -ii) a progressive decrease of the calculated strength as a function of the flattening rate, independent of the
290 initialization strength.

291 We ran different simulations using varied pyroxenes mixture spectra and olivine alone spectra. In
292 this paper, we only display the example resulting of the simulation based on the
293 orthopyroxene/clinopyroxene mixture spectrum mentioned above. Figure 3-B represents the final center
294 positions (i.e., after running the MGM) of the two orthopyroxene Gaussians in the 1 (left) and 2 (right)
295 μm domains. For both diagrams, one can clearly note variations across the parametric space. In the 1 μm
296 domain, the center position presents a 180 nm difference between the maximum and the minimum values.
297 The lowest center is found when a flat spectrum is modeled with high initial strength; conversely the
298 highest center is found when a spectrum showing well defined absorptions is modeled with low initial
299 strength. The overall regular spacing between two contiguous contour lines indicates a progressive shift.
300 In the 2 μm domain, the center final position varies between 1600 and 1850 nm, following a similar trend
301 to the 1 μm domain. One should note however that beyond a particular ratio between the initial Gaussian
302 strength and the strength of the absorption, values of the center final position are more stable (upper left
303 part of the diagram). Though not shown here, results in the case of clinopyroxene Gaussians show

304 basically a similar behavior, with a reversed trend, i.e. the highest center positions are associated with a
305 flat spectrum combined with high initial strength.

306 The calculated Gaussians strength evolution has also been documented (see graphs on figure 3-C).
307 Contour lines can be separated in two areas, the limit being the first diagonal of the graph. In the upper
308 left triangle, contour lines are closer to horizontal and regularly spaced out. It means that, independently
309 of the initialization, final Gaussians strengths are only function of the flattening rate, i.e. the strength of
310 the mineralogical absorption. On the other hand, in the lower right triangle part of the graph, contour lines
311 are curved downward and tend to be vertical, which implies that this time the final Gaussians strengths
312 are only function of the initialization strength. Similar trends are once again observed in the case of
313 clinopyroxene Gaussians. Those results highlight that for both centers and strengths, a special attention
314 must be put on the initialization of Gaussians parameters. Similar conclusions are drawn when different
315 orthopyroxene/clinopyroxene ratios and various grain sizes are considered on the basis of the Sunshine
316 and Pieters (1993) set of spectra.

317 A series of olivine spectra from the Sunshine and Pieters (1998) set has also been
318 examined. It is found that the results are less dependent on the initialization setting. Final centers appear
319 to be shifted only when the flattening rate and the initial strength are high. In such case, as for pyroxenes,
320 results cannot be related to mineralogical information.

321 The last aspect of our assessment deals with the uncertainties on the initial strength parameters
322 and shows that a variation of these uncertainties has no major influence on the MGM deconvolution
323 process. In the following, these uncertainties will be taken such as they will be an order of magnitude
324 larger for band centers, on the same order for band widths, and an order of magnitude less for band
325 strengths than in earlier studies (Sunshine and Pieters, 1993; Sunshine et al., 1998). These results suggest
326 that one may relax the constraints set on the band center without doing any harm to the solution.

327 In conclusion, this section shows that the MGM initialization phase cannot be carried out in a
328 blind way and that the MGM modeling cannot be used automatically on a complex data set (e.g. airborne
329 or orbital data) without some careful settings. As an example, data from Sunshine and Pieters (1993)
330 indicate that the orthopyroxene endmember absorptions are located around 907 and 1827 nm (represented
331 by dashed lines on Fig.3). These results can only be obtained with specific combinations of the initial
332 Gaussians strength versus the flattening rate (e.g. for a 50% flattening rate, strength initialization should
333 be close to -0.30 while for a 80% rate, it should be close to -0.12). For too weak absorptions (simulated
334 by a flattening rate of 80% or more), it may happen that the MGM deconvolution returns results unrelated
335 to the mineralogical information. This case apart, a first-order linear relation is found between the two
336 parameters. This fact will be used in the next section to automatically initialize the MGM.

337

338 2.2.3 Automatic initialization of the Gaussians parameters

339

340 Considering a spectrum of an unknown mafic assemblage, one cannot choose a priori a given
341 mineralogical configuration among the seven possible ones. The first step of our automatic initialization

342 consists in the analysis of the spectrum global shape (cf. section 2.2.1). The spectrum maxima and
343 minima are used to estimate the measured absorption strengths and widths (Figure 2), with the strength
344 estimate defined as the difference between the reflectance minimum and a straight line linking the
345 adjacent maxima and the measured width estimate defined as the width at half strength. As a result, the
346 general characteristics of a spectrum can be described by four parameters. The next step of the
347 initialization is then to link for a given mineralogical combination those parameters to expected values for
348 the Gaussians as defined in the literature.

349 As we consider the seven possible mineralogical associations, the meaning of the four measured
350 parameters may differ. In the case of a single pyroxene, interpretation is easy as each Gaussian is directly
351 related to the combination of the measured strength and width. In the case of olivine, the three Gaussians
352 overlap and the case appears more complex. However, results from Sunshine and Pieters (1998)
353 established relationships between the three Gaussians. On this basis of knowledge, a partitioning is made
354 between the Gaussians, the strength and width of Gaussians “850” and “1050” being calculated as a
355 function of the “1250” one for which parameters initialization depends on the 1 μm measured absorption
356 feature and on the Sunshine and Pieters (1998) results.

357 In the case of a pyroxene mixture, several steps must be used. Indeed, whatever the pyroxene
358 composition, Gaussians in the 1 μm and 2 μm domains overlap without obvious relationships. First, a first
359 order linear approximation is drawn between the position of the reflectance minimum in the 1 μm domain
360 and the mixture composition. This is established on the basis of the Sunshine et al. (1993) dealing with
361 seven compositions and three grain sizes. In a second step, we calculate from the results of the literature
362 the relative strength of the orthopyroxene Gaussian compared to the clinopyroxene one in the 1 μm
363 domain. Figure 4-A shows that the relation is non-linear, orthopyroxene strength being generally more
364 important than the clinopyroxene strength. In addition, one notes that when orthopyroxene represents
365 more than 65% of the mixture, the grain size has a drastic effect on the OPX/CPX strength ratio. To take
366 into account those constraints, the choice has been made to split the mixture composition range in five
367 intervals (below 10% of orthopyroxene, only clinopyroxene absorptions can be resolved, while above
368 90% of orthopyroxene, only orthopyroxene absorptions can be resolved). For each of them, a
369 characteristic ratio is fixed and will be used further (e.g. Cpx strength/Opx strength ratio varies from 2/1
370 to 1/12, see Figure 4-A for details). At this time, the relative strength parameters are settled in the 1 μm
371 domain. We now have to link the orthopyroxene Gaussian strength defined by Sunshine and Pieters
372 (1993) and the absorption feature strength measured on the spectrum. Such a relation can be
373 approximated to first-order by a linear regression, with some fluctuations caused by grain size effects.
374 This relationship permits us to initialize efficiently the different Gaussians. Finally, a ratio, based on
375 Sunshine and Pieters (1993) results, is defined which permits us to initialize the 2 μm Gaussians band
376 strength as a function of the 1 μm Gaussians band strength (Figure 4-B). These empirical ratios
377 (opx_1/opx_2 , cpx_1/cpx_2) are determined within five distinct intervals of mixture composition for both ortho-
378 and clinopyroxene, respectively (see Figure 4-B). As a result, all the Gaussian strengths in the 1 and 2 μm

379 domains can be initialized from one measured parameter on the spectrum that is the depth of the 1 μm
380 feature. A similar approach is developed for the width parameters.

381 For olivine-pyroxene mixtures, no systematic study of the MGM behavior as a function of the
382 relative proportions of the mineral constituents is available so far to initialize the Gaussians parameters.
383 For the olivine-orthopyroxene mixture, we used a set of 5 spectra found in the RELAB library (from
384 Mustard and Pieters (1989) and Hiroi and Pieters (1994) (see also in section 3.2.1)). Thus, Gaussians
385 parameters calculated by the MGM for a mineral alone are used as a reference in the mixture case. Then,
386 the steps described for the pyroxene mixtures are repeated with the introduction of the three coupled
387 Gaussians in the 1 μm domain for the olivine as detailed above. Next, we extrapolate those new results to
388 olivine-clinopyroxene mixtures. We here used a set of spectra acquired on the field in Oman's ophiolite
389 with an ASD FieldSpec[®] 3 field spectrometer. They do not span however the full range of
390 olivine/clinopyroxene possible mixtures and are mostly used as a first-order estimate to calibrate the
391 Gaussians parameters. Finally for the most complicated case (ternary mixtures of olivine-orthopyroxene-
392 clinopyroxene), our experimental knowledge is limited as it relies on only three spectra of identical
393 composition, with various grain sizes (spectra from Mustard et al. (1993) and Pieters et al. (1993)).
394 Following Ockham's razor principle, all the Gaussian functions associated with the three minerals are
395 initialized with an identical strength defined as one third of the measured depth of the 1 μm absorption
396 feature of the spectrum.

397 The stability of the automatic initialization is assessed as previously demonstrated (see Fig. 3).
398 MGM calculated parameters are directly plotted as a function of the flattening rate. Shown on Figure 5
399 are the results for a 50/50 pyroxene mixture (left) and 75/25 olivine-orthopyroxene mixture (right). We
400 can see that for a flattening rate less than 80% those results are quite stable for center parameters,
401 meaning that the case of very shallow absorption features excepted (which may require to set some
402 threshold when dealing with an hyperspectral image), the MGM deconvolution is able to extract the
403 mineralogical information. Figure 5 also shows that final Gaussians strengths vary linearly as a function
404 of the flattening rate. However, as found in the case of Gaussian centers, when the absorption is too weak,
405 parameters estimates should be taken cautiously. These situations set aside, our automatic initialization is
406 able to process a wide range of natural spectra, with promising applications on large datasets.

407
408 2.2.4 Mineralogical sorting

409
410 As explained earlier, we run successively on an unknown spectrum the MGM with the seven
411 configurations in order to test every possible combination of the three mafic minerals. Root-mean-square
412 (*rms*) between model and observation is used as a mandatory convergence criterion. However, the
413 potentially large number of Gaussian functions may result in low *rms* mathematical solutions without
414 physical meaning. The next simple criterion consists in the rejection of solutions with positive band
415 strengths (i.e., associated with spectral features "above" the continuum) indicative of a wrong modeling
416 (due to the use of too many Gaussians for instance versus the number of real absorptions). The retrieved

417 mathematical solutions have then to be assessed on spectroscopic grounds and accordingly either
418 validated or discarded. This final step is accomplished through a mineralogical sorting of the returned
419 MGM results, keeping in mind that the modeled Gaussian functions must verify spectroscopic criteria to
420 be validated in view of a mineralogical interpretation. As an example, for olivine, our MGM results show
421 that the position of the three centers increases to longer wavelength with higher Fe content, as established
422 in Sunshine et al. (1998). So, each Gaussian function must have its center between the minimum and the
423 maximum values (e.g. between 0.81 μm and 0.94 μm for the “850” Gaussian). Similarly, the band widths
424 have to satisfy to the experimental constraints set by Sunshine and Pieters (1998), with some margin
425 based on the MGM uncertainties as defined by Kanner et al. (2007) and on the diversity of the laboratory
426 spectra we have studied ourselves, including olivine with larger grain size and olivine/pyroxenes
427 mixtures. Constraints on the relative strength of the different Gaussian functions are also used knowing
428 that the “1250” absorption is always stronger than the “850” and “1050” ones (Sunshine and Pieters,
429 1998). Only if all those criteria are satisfied, can the MGM solution be validated as an indication of the
430 presence of olivine.

431 We used the same approach in the case of pyroxene absorptions, relying on Adams (1974) and
432 Sunshine and Pieters (1993) experimental data. For pyroxenes, in addition to the previous constraints, we
433 add an additional rejection criterion based on the fact that the 1 and 2 μm absorption positions are coupled
434 as shown by Adams (1974). However, it is to be reminded that pyroxene is a solid solution, with the
435 implication that intermediate pyroxenes may present absorption features that can be interpreted both in
436 terms of orthopyroxene and clinopyroxene. Moreover, minor amounts of elements such as Ti can modify
437 the relative absorptions centers in the two wavelength domains, shifting the pyroxene position above
438 Adams (1974) trends (Cloutis and Gaffey, 1991).

439 At the end of the mineralogical sorting process, three situations can occur:

- 440 -i) First, all the solutions are rejected. This means that either there are no mafic minerals in the analyzed
441 rock or there is an additional spectrally active mineral which is not taken into account by our systematic
442 procedure.
- 443 -ii) only one configuration matches all the constraints: this mathematical solution is physically realistic
444 and Gaussian function parameters can be used to extract minerals characteristics.
- 445 -iii) two (or rarely more) configurations can be accepted. This effect depends on the characteristics of the
446 minerals relative absorptions. For instance, pyroxene absorptions may hide olivine ones and in the case of
447 a 50/50 olivine-orthopyroxene mixture, it appears that two configurations are validated (see Figure 6), all
448 the other configurations being rejected as they fail at modeling properly the spectrum or they do not
449 satisfy spectroscopic criteria associated with olivine and /or orthopyroxene mineral(s). When at least two
450 configurations are kept, we will consider the most complicated mixture as the most representative to
451 identify the presence of minerals.

452 In the first part of the paper, the implemented procedure has been described. In the following, it
453 will be applied on different laboratory spectra to test its ability for:

- 454 -i) the detection of the presence of mafic minerals in a given assemblage;

455 -ii) the characterization of their chemical compositions.

456

457 3. Results

458

459 3.1 Case of simple mafic mineralogies

460

461 3.1.1 Olivine

462

463 Our approach is first validated in the case of olivine alone, using a set of 28 spectra from the
464 RELAB library (cf. Table 2). Ten of them were used by Sunshine and Pieters (1998). The present set
465 deals with a larger spectral variety than in Sunshine and Pieters (1998), both in terms of mean reflectance
466 level and relative strength of the absorptions. Our systematic approach, including the seven
467 configurations, has been applied to all spectra and in each case, only the olivine configuration is retained.
468 MGM results are given (Fig. 7) for three compositions ($\text{Fo}_{96.9}$, $\text{Fo}_{50.5}$, $\text{Fo}_{0.1}$) spanning the whole range of
469 the solid solution.

470 Gaussian function parameters are in general agreement with the trends defined by Sunshine and
471 Pieters (1998), with widths and normalized strengths corresponding to those defined in the literature. As
472 expected, both an increase of the Gaussian centers positions toward longer wavelengths correlated to the
473 iron content and of the “1050” normalized intensity are observed. However, due to the choice of a second
474 order polynomial continuum, weaker strengths in the case of the Gaussian “850” (i.e. between -0.4 and -
475 0.6) are obtained. Indeed, the continuum presents a tight curvature at shorter wavelengths and thus better
476 matches the overall shape of the spectrum than in the case of a straight line, with an effect on the relative
477 “850” and “1050” strengths. Evolution of the three Gaussian centers position as a function of iron content
478 is similar to Sunshine and Pieters (1998) results. However, the definition of a second-order polynomial
479 continuum slightly modifies the relations established for the Gaussians center position. Accordingly, the
480 three regression lines established by Sunshine and Pieters (1998) have been recalculated in order to derive
481 the composition of an unknown olivine. The band center position for the “1250” Gaussian appears to be
482 shifted by a few nanometers toward longer wavelengths with basically the same slope coefficient as in
483 Sunshine and Pieters (1998).

484 Our work on laboratory data shows that olivine can be properly detected and compositionally
485 characterized. However, when dealing with natural conditions, grains size may also affect the chemical
486 characterization (e.g. Crown and Pieters, 1987; Mustard and Hays, 1997; Lucey, 1998). Results on Figure
487 8 (left) show indeed that large grains size forsterite have absorption characteristics that may mimic
488 fayalite absorption features. This effect, not really documented in the literature, appears when the grains
489 size exceeds 250 μm and for grains larger than 1 mm, approaching the case of rock slab, saturation may
490 be reached (e.g., Pompilio et al., 2009). In this situation, MGM results can be ambiguous and large grain
491 size forsterite might be interpreted as fayalite (Fig. 8 right). Consequently, interpretation of MGM results
492 when considering an unknown olivine must be carefully taken. Indeed, in the absence of grain size

493 knowledge, olivine could have a lower Fe content than predicted by remote sensing, with significant
494 implications (e.g., Poulet et al., 2009a).

495

496 3.1.2 Pyroxenes

497

498 The case of monomineral pyroxenes is then examined for the purpose of validation. We used a set
499 of 19 spectra from the RELAB library. Twelve of them, the synthetic orthopyroxene suite (enstatite-
500 ferrosilite), were used by Klima et al. (2007). Other spectra present various compositions of natural
501 pyroxenes ranging from enstatite to diopside and hedenbergite (RELAB spectra references are mentioned
502 throughout the paper). Our systematic approach with seven configurations (cf. Table 1) has been applied
503 on the entire set. In most cases, only one mathematical solution issued for either orthopyroxene or
504 clinopyroxene configuration is retained. Figure 9 shows the MGM results for four compositions. One
505 should note that in the case of an intermediate pyroxene, e.g. with a pigeonite, both opx and cpx
506 configurations give similar mathematical solutions, consistent with the fact that the position of the band
507 centers associated with orthopyroxene and clinopyroxene may overlap each other (Adams, 1974).

508 For almost all the pyroxenes investigated here, the present MGM outputs are in agreement with
509 earlier results in the literature. However, for three spectra of our set, none of the seven mathematical
510 solutions corresponds to the expected trends. Those spectra are associated to hedenbergite, a Fe- and Ca-
511 rich pyroxene (in our case compositions are respectively $Wo_{49}En_4Fs_{47}$ (RELAB C1PP12), $Wo_{55}En_9Fs_{36}$
512 (RELAB C1PP14) and $Wo_{53}En_2Fs_{45}$ (RELAB C1SB15)), and correspond to spectral type A
513 clinopyroxenes (Wo close to or greater than 50 mol %; Cloutis and Gaffey, 1991). Indeed, as mentioned
514 previously, such minerals show a very strong absorption in the 1 μm domain with no absorption (or a
515 very subdued one) in the 2 μm domain. Schade et al. (2004) have shown that three dedicated Gaussian
516 functions, different from olivine ones, are then needed to model the 1 μm feature and no configuration
517 has been developed and tested so far in our approach to handle this case.

518 With this limitation in mind, we assess the performance and consistency of the MGM outputs
519 versus Adams (1974)'s results. First, one explores the spectral evolution associated with an iron content
520 variation in the case of a synthetic orthopyroxene series (Klima et al., 2007). For enstatite, absorptions are
521 centered around 900 and 1800 nm while they are centered around 920 and 1960 nm for $En_{50}Fs_{50}$ and 940
522 and 2070 nm for ferrosilite. A progressive shift (Fig. 10-A) of the Gaussians center toward longer
523 wavelengths is obtained in general agreement with the literature (Adams, 1974; Hazen et al., 1978;
524 Cloutis and Gaffey, 1991). This effect is particularly pronounced for the 2 μm absorption (Figure 10-A).
525 Moreover, a linearly coupled behavior is found between the 1 and 2 μm Gaussians strength, i.e. when the
526 1 μm absorption gets stronger, the 2 μm one also increases in proportion, as expected. The "1200"
527 Gaussian strength also increases when dealing with high Fe orthopyroxene (Fig. 9-A right).

528 Analysis of various natural pyroxenes spectra (Fig. 10-B) show that compositions close to
529 endmembers (diopside or enstatite, respectively dots 1-2 and 3-4) have absorption centers similar to those
530 found by Adams (1974). For intermediate composition pyroxenes, the case of augite (dot 6) falls well in

531 the pyroxene general trend while pigeonite (dot 5) may depart a bit from it. It could be the case with a
532 zoned pyroxene, or in the presence of minor elements such as Ti (Cloutis et al., 2002). Pigeonite is
533 frequently exsolved and/or inverted to orthopyroxene and it may result in a complicated mineralogical
534 texture. Such effects are not yet clearly documented in the literature.

535 The confrontation of our results with Adams (1974) trends shows that our systematic MGM
536 deconvolution returns a reliable piece of information about the pyroxene type. The next step is to assess
537 how precisely the pyroxene chemical composition can be estimated. To do that, we use data from Hazen
538 et al. (1978) and Cloutis and Gaffey (1991) which documented the evolution of the absorption centers as
539 a function of the Ca and Fe content in the pyroxene quadrilateral. RELAB chemical analysis and literature
540 data have been used to plot the pyroxenes (with colored circles) in the four graphs on Figure 11. Red
541 contoured circles correspond to the set of synthetic orthopyroxenes (Klima et al., 2007) while the blue
542 contoured circles are associated with the various natural pyroxenes described in the previous paragraph.
543 Colors within the circles and in the background correspond respectively to the absorption center position
544 obtained by our approach, and to the determinations found by Hazen et al. (Fig. 11 left) and Cloutis and
545 Gaffey (Fig. 11 right). That way, if the MGM result is in agreement with literature data, the color inside
546 the circle must be the same as the surrounding background color. An overall excellent agreement is found
547 in the case of the suite of synthetic orthopyroxenes as the Fe content varies from 0 (En case) to 100% (Fs
548 case). Our results fit both Hazen et al. and Cloutis and Gaffey data. However, for Ca-rich pyroxenes,
549 discrepancies are observed and our results appear to fit better Cloutis and Gaffey values. In particular,
550 band center positions produced for the three clinopyroxene spectra are at variance with Hazen et al.
551 values, both at 1 and 2 μm . As it stands, we can estimate a range of composition for an unknown
552 pyroxene but not determine very accurately its location in the quadrilateral. Interestingly, going back to
553 the case of the diopside shown on Figure 1, band centers positions found by MGM deconvolution are
554 very consistent for the three powder spectra (1.019 and 2.290 μm for spectrum A, 1.016 and 2.294 μm for
555 spectrum B and 1.017 and 2.307 for spectrum C) and for the three rock spectra (1.044 and 2.266 for
556 spectrum 1, 1.043 and 2.298 for spectrum 2 and 1.038 and 2.253 for spectrum 3).

557 We also test the capability of our approach to deconvolve pyroxenes mixtures spectra. We here
558 used the set from Sunshine and Pieters (1993). Mixture composition evolves progressively between 100%
559 diopside and 100% enstatite, for three grains size ranges (<45 μm , 45-75 μm and 75-125 μm). The results
560 are illustrated with the case of the less than 45 micron particles suite. Our systematic approach, including
561 the seven configurations, has been applied on the complete set. The configuration(s) validated for each
562 mixing case is (are) reported in Table 3, and the band center positions found at 1 and 2 μm (Fig. 12) are
563 compared to the pyroxene trend defined by Adams (1974). As one could expect, endmembers are
564 modeled by the corresponding appropriate configuration, i.e. either the orthopyroxene or clinopyroxene
565 one. In the case of mixtures, different situations may occur depending on the mixture, and the grains size
566 which modifies the strength and width of the absorptions. Indeed, it is noted that an orthopyroxene will
567 mask clinopyroxene absorptions more easily when dealing with large grains size. However, the general
568 rule is that a mineral which is clearly dominant in the mixture (>75%) is detected by its dedicated

569 configuration. Then in the case of intermediate mixtures, both the two-components and the dominant
570 pyroxene configurations are validated. In this situation, as defined in the section 2.2.4, the two-
571 components mixture has to be considered as the most representative for detecting the minerals in
572 presence. Conversely, one must bear in mind for the sake of interpretation that below a given critical
573 threshold, a mineral in too weak a proportion may not be detected.

574 Also, a result of note is to highlight the fact that the band center determination from MGM
575 deconvolution is more accurate in the 1 μm domain than in the 2 μm domain. This may be the result of an
576 indirect edge effect on the continuum caused by the spectral truncature at 2600 nm. Consequently, a more
577 reliable estimation of the pyroxene chemical composition in mixtures situations will be returned from the
578 1 μm Gaussians.

579

580 3.2 Olivine-pyroxene mixtures

581

582 3.2.1 Olivine, orthopyroxene without / with plagioclase

583

584 As described previously, a number of studies dealing with simple mineralogies exist in the
585 literature. However, there is a lack of quantitative assessment that we address here, concerning the MGM
586 ability to model olivine-pyroxene(s) mixtures spectra. For this purpose, a set of spectra dealing with
587 binary mixtures of olivine (Fo_{90}) and low-calcium pyroxene (hypersthene) ranging from (10% Ol, 90%
588 LCP) to (90% Ol, 10% LCP) (referred to as C1AG14, and C1AG17 to C1AG20 in the RELAB
589 collection) has been used first. Then, a dedicated set of spectra (Mustard and Pieters, 1989; Hiroi and
590 Pieters, 1994) with different amount of olivine (Fo_{85-89}), orthopyroxene (En_{85-90}) and plagioclase
591 ($\text{An}_{78}\text{Ab}_{22}$) has also been analyzed (cf. Table 4). With this approach, the effect on the deconvolution
592 process of the plagioclase considered as an optically neutral mineral can also be tested.

593 Our systematic approach, including the seven configurations, has been applied to the complete set.
594 As an example of deconvolution, MGM outputs produced in the case of the O150/Opx50 mixture are
595 displayed on Figure 6. The configurations kept for each spectrum are reported in Table 4. First, our
596 approach is tested on a pure plagioclase spectrum. Results show logically that no solution among the
597 seven mafic configurations is validated. For all other spectra, the only validated configurations involve
598 either olivine, orthopyroxene or both minerals. First binary mixtures, involving plagioclase and a mafic
599 mineral are considered. Whatever the abundance of plagioclase, the configuration which is validated
600 corresponds to the proper monomineral one (olivine or orthopyroxene), showing that in these situations
601 the MGM deconvolution is not hampered or biased by the presence of an optically neutral mineral. This
602 point will be confirmed in the following in the case of ternary mixtures, involving both olivine and
603 orthopyroxene.

604 Then, Table 4 shows the results when considering ternary mixtures (binary mixtures of olivine and
605 orthopyroxene, with a variable amount of plagioclase). Depending on the olivine/orthopyroxene content,
606 three situations are encountered. First, when orthopyroxene is the dominant mineral (more than 72%

607 relative to olivine), only its configuration is kept which means that in this context the presence of olivine
608 may not be detected, even if the global shape of the spectra is slightly modified. In fact, the “1200”
609 Gaussian center may be shifted to longer wavelengths, which can be used as an indicator of the olivine
610 presence (Parente and Bishop, 2006). A second situation is found when olivine and orthopyroxene are in
611 the same proportion. Then, two configurations are kept: the orthopyroxene one and the olivine-
612 orthopyroxene mixture one, even with only 16% of each mineral in the mixture composition. As
613 explained earlier (see section 2.2.3 and Fig. 6), the most realistic detection is then provided by the most
614 complex configuration (see Fig. 6). Finally, if olivine represents more than 72% relative to
615 orthopyroxene, only the mixture configuration is validated. We verify here that when the olivine or
616 orthopyroxene is the respective dominant mineral, their absorption bands do not play a symmetrical role
617 (i.e., for $Opx/Ol > 72\%$, orthopyroxene configuration is found while for $Ol/Opx > 72\%$, olivine-
618 orthopyroxene configuration is found) as it was recognized long ago (e.g., Singer, 1981). In conclusion,
619 considering the detection capability of our approach, we note that the presence of olivine can be detected,
620 even when this mineral is not clearly dominant in the mixture. Conversely, this test also shows that some
621 care must be put in the interpretation as when a mineral is not detected, it does not necessarily mean that
622 it is not present in the mixture.

623 Based on those detections, Gaussians parameters can be used to derive the minerals chemical
624 composition in the case of mafic mineralogies. However, to correctly interpret the centers positions,
625 verification is needed to assess their stability as a function of the minerals content in the case of complex
626 mixtures.

627 Concerning the band center position of the orthopyroxene Gaussians, the deconvolution process is
628 logically not affected at 2 μm by the presence of olivine, whatever its proportion (Fig. 13). The
629 orthopyroxene 1 μm band center position appears also very stable as long as the olivine relative
630 proportion is less than 70% in the mixture (Fig. 13). The most critical cases arise when the proportion of
631 Opx is low versus Ol+plagioclase (cases of RELAB C1XT32, C1XT 33, C1XT 38). A moderate shift to
632 longer wavelengths on the order of 30 nm is then observed. It suggests that a plagioclase absorption
633 should then be considered in the present MGM modeling and this limitation must be kept in mind for the
634 matter of interpretation.

635 Then, considering the “850”, “1050” and “1250” olivine Gaussians, they present band center
636 positions which are well determined, for olivine proportions exceeding 50%, and are consistent with the
637 respective Fo_{85-90} and Fo_{90} compositions of the samples used here. For lesser proportions, the “1050”
638 appears shifted to longer wavelength and is thus not well determined. In these cases, the ‘OPX’
639 configuration is also validated by the MGM modeling, consistent with the fact that in the case of minor
640 proportions of olivine, its detection may be difficult. Though not perfect, these results show that an
641 olivine-pyroxene MGM deconvolution is operational with our approach, and that at least a first-order
642 assessment of the olivine type (i.e. forsterite, fayalite or intermediate compositions) is possible, not
643 excluding a more quantitative estimate in terms of olivine composition.

644

645 3.2.2 The most complicated case: an example of ternary mixture of mafic minerals

646

647 The case addressed here consists in a mafic ternary mixture (i.e. olivine, orthopyroxene and
648 clinopyroxene). We consider three spectra of the same composition (20% olivine, 20% orthopyroxene and
649 60% clinopyroxene; RELAB C1XS01, C1XS02, C1XS03) (Mustard et al., 1993; Pieters et al., 1993),
650 referred to as A, B, C in the following. Each mineralogical phase has been separated in three grain sizes
651 ($S < 25 \mu\text{m}$, M between 25 and 75 μm , L between 75 and 250 μm) and three soils have been created: SS
652 (65% S, 25% M, 10% L), MS (25% S, 50% M, 25% L) and LS (10% S, 25% M, 65% L). Details on
653 spectra A, B, C and RELAB references can be found in Table 5.

654 The seven configurations, automatically initialized, have been applied on these three spectra and
655 the results are given in Table 5 and figures 14, 15. It is found that four configurations can provide a
656 realistic modeling. However, despite the fact that the CPX configuration is capturing most of the essence
657 of the first-order spectral characteristics (see Fig. 14-A), the successive configurations: 'CPX-OPX',
658 'CPX-OL', and 'CPX-OPX-OL' improve increasingly the modeling as shown by the rms residuals (0.005
659 down to 0.0025). As noted earlier, the most complex configuration provides the best description in terms
660 of minerals detection. Interestingly, while it is not the case with the 'CPX-OPX' configuration, the
661 Normalized Band Strength Ratio (NBSR) introduced by Kanner et al. (2007) returns consistent values
662 both at 1 and 2 μm in the case of the 'CPX-OPX-OL' configuration.

663 Those tests on ternary mixtures are not yet complete and beyond this first exploration, a more
664 extensive study remains to be carried out. However, with this new procedure, modeling of complex
665 spectra is no longer out of reach, and the handling of weak spectral signatures requiring an increasing
666 number of Gaussians appear tractable.

667

668 4. Conclusion

669 Our work shows that this new MGM approach is able to model simple and complex mafic
670 mineralogies, including binary and ternary mixtures, for a large range of grain sizes. A key issue is to
671 initialize the MGM procedure with a proper setting for the Gaussians parameters, relying on an automatic
672 analysis of the shape of the spectrum and on the basis of laboratory results available in the literature in the
673 case of simple mixtures of mafic minerals. The continuum is then handled with a second order
674 polynomial adjusted on the local maxima along the spectrum and permits us to address the case of
675 laboratory (controlled powders) and natural rock spectra. The procedure implemented here considers all
676 the mixture possibilities involving orthopyroxene, spectral type B clinopyroxene and olivine and use
677 accordingly for each configuration different numbers of Gaussians, depending on the potential complexity
678 of the mixture. This systematic search is quite efficient to deal with an a priori unknown mafic
679 mineralogy observed in the visible-near infrared by reflectance spectroscopy, as it is frequently the case
680 with hyperspectral orbital data sets.

681 The results presented in this paper are a quantitative step forward to characterize both modal and
682 chemical compositions of pyroxenes and olivines. A demonstration of the methodology on specific

683 examples of binary and ternary olivine-pyroxenes mixtures (with and without plagioclase) has been made,
684 which shows that the different non-linear effects which affect the Gaussian parameters (center and
685 strength) can be successfully handled. Of note is the fact that the band center positions associated with the
686 different mafic minerals are not predetermined here in the inverse problem, and thus the MGM outputs
687 are truly informative of the chemical composition of pyroxenes and olivines, keeping in mind that large
688 grains size forsterites have absorption characteristics that may mimic fayalite absorption features. With
689 the consideration of some limits on the detection thresholds, these results are quite promising for
690 increasing the operational use of the Modified Gaussian Model with large hyperspectral data sets, for
691 establishing detailed lithological/mineralogical mappings intended to explore the petrology and
692 geological history of magmatic units (e.g., Bibring et al., 2006; Mustard et al. 2005; Baratoux et al., 2007;
693 Mustard et al. 2007; Combe et al., 2008; Poulet et al., 2009b; Clenet et al., 2010; ...). However, to go
694 further in this work, spectra with a wider range of compositions should be studied, including a variety of
695 pyroxenes chemical compositions and olivine-pyroxene(s) mixtures, in order to thoroughly assess the
696 thresholds of detection and limits on the components quantification. Ultimately, building on the present
697 learning, the use of mineralogical constraints bearing for instance on the coupling of the 1 and 2 micron
698 pyroxene absorptions or on the olivine absorptions, should be set in the correlation matrix to be directly
699 accounted for in the process of the inversion.

700

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892 Figures captions

893

894 Tab. 1

895 Gaussians present in the different configurations, with Ol for olivine, Opx for orthopyroxene and Cpx for
896 clinopyroxene (spectral type B). Gaussians are named by the position of their center. An “X” means that
897 the Gaussian is used in the corresponding configuration.

898

899 Tab. 2

900 Suite of 28 olivine spectra used, spanning the whole range of composition from Fo_{0.1} to Fo_{96.9}, with
901 variable grain sizes. Rms estimates indicate the quality of the spectral fit obtained with the olivine
902 configuration.

903

904 Tab. 3

905 Summary of the retained configurations as a function of the relative abundance of diopside and enstatite
906 in the mixture. Endmembers are modeled with one configuration only while mixtures can be correctly
907 modeled with one or two configurations. As explained previously in the text, when two configurations are
908 validated the most complex one should be used to extract chemical compositions (see text for details).
909 Rms estimates indicate the quality of the spectral fit.

910

911 Tab. 4

912 Summary of the retained configurations as a function of the abundance of olivine, orthopyroxene and
913 plagioclase in the mixture (grains size: 45-75 μ m). Rms estimates indicate the quality of the spectral fit.

914

915 Tab. 5

916 Summary of the performances associated with each configuration for the three investigated spectra
917 involving a ternary mafic mixture (Opx, Cpx, Ol). Rms estimates indicate the quality of the spectral fit
918 associated with the retained configuration(s).

919

920

921 Fig. 1

922 Differences between powder spectra (labeled A ($0 < \emptyset < 45 \mu\text{m}$), B ($45 < \emptyset < 75 \mu\text{m}$), C ($75 < \emptyset < 125 \mu\text{m}$))
923 acquired in laboratory (dashed lines) and natural rocks spectra (labeled 1, 2, 3) we acquired during a field
924 campaign in Oman with an ASD FieldSpec[®] (plain lines). All the spectra correspond to clinopyroxene
925 (diopside: powder $\text{Wo}_{46}\text{En}_{46}\text{Fs}_9$; rock: $\text{Wo}_{48}\text{En}_{47}\text{Fs}_5$) with almost the same chemical composition
926 (RELAB database and microprobe analysis). One can see that field spectra show less pronounced
927 absorption bands and a lower reflectance mean level.

928

929 Fig. 2

930 Parameters used to define a spectrum global shape. In this example, the spectrum is an olivine-
 931 orthopyroxene mixture (respectively 75% and 25%) from the RELAB spectral library.

932

933 Fig. 3

934 a) Variations of the absorptions strengths simulated by an artificial flattening of a laboratory spectrum
 935 (mixture of 40% Opx and 60% Cpx). 0% corresponds to the reference spectrum from RELAB library.
 936 Absorptions characteristics are modulated from 0 to 100%, i.e. a perfectly flat spectrum. b) Final center of
 937 the orthopyroxene gaussians (color [or grey] scale) as a function of the initialization strength (horizontal
 938 axis) and the flattening of the spectrum (vertical axis). Dashed lines defined an area corresponding to the
 939 values given by Sunshine and Pieters (1993), taking into account for the variability defined by Kanner et
 940 al. (2007). c) Final strength of the orthopyroxene gaussians (color [or grey] scale) as a function of the
 941 initialization strength (horizontal axis) and the flattening of the spectrum (vertical axis).

942

943 Fig. 4

944 Relations between parameters defined in Fig. 2; mixture characteristics and Gaussians parameters as
 945 calculated by Sunshine et al. (1993) for this set. We use spectra from the RELAB library, considering a
 946 two-pyroxene mixture (100% clinopyroxene to 100% orthopyroxene) with three grain size (<45 μ m
 947 (displayed with black dots), between 45 and 75 μ m (displayed with dark grey dots) and between 75 and
 948 125 μ m (displayed with light grey dots)). Diagram a: Ratio between the Gaussians strength of the two
 949 pyroxenes calculated by Sunshine et al. and the mixture composition, estimated from the first step of our
 950 approach (see text); Diagram b: relation between the Gaussians strength of a given pyroxene (opx or cpx)
 951 at 1 and 2 micron as a function of the orthopyroxene proportion in the mixture composition (black square
 952 corresponds to 1 micron opx band strength, black star to 2 micron opx band strength, grey square to 1
 953 micron cpx band strength, grey star to 2 micron cpx band strength, black triangle to the ratio of the 1 μ m
 954 opx band strength/ 2 μ m opx band strength (opx_1/opx_2), grey triangle to the ratio of the 1 μ m cpx band
 955 strength/ 2 μ m cpx band strength (cpx_1/cpx_2)). In both diagrams, five intervals separated by vertical
 956 dashed lines are defined as a function of the mixture composition. For each interval, empirical
 957 coefficients have been defined (see text) (e.g., in diagram a, Cpx strength/Opx strength ratio is
 958 successively equal to 2/1, 1/1, 1/2, 1/12, 1/12; in diagram b, opx_1/opx_2 is equal to 1.7, 1.5, 1.5, 1.4, 1.35
 959 and cpx_1/cpx_2 is equal to 3.08, 2.92, 2.76, 2.58, 2.45). The two hatched black and grey lines visualize the
 960 result of the linear regressions for opx and cpx, respectively.

961

962 Fig. 5

963 Calculated Gaussians parameters obtained with the automatic initialization. Tests with synthetic spectra
 964 are similar to the tests described in Fig. 3. Pyroxenes mixture results are represented on the left side while
 965 olivine-orthopyroxene mixture results are represented on the right side. From top to bottom, parameters
 966 considered are the band center positions, strengths for all the Gaussians.

967

968 Fig. 6

969 MGM Analysis of a 50/50 olivine-orthopyroxene mixture spectrum (RELAB C1XT31). Shown on each
970 graph are the measured spectrum, the spectral position of the local maxima along the spectrum used for
971 the process of initialization (see section 2.2), the MGM modeled spectrum with the Gaussians and
972 polynomial determined by the MGM deconvolution and the residuals line along the spectral domain.
973 Gaussians are displayed with a solid black line for orthopyroxene and a dotted grey line for olivine. Solid
974 grey line corresponds to Gaussian "1200". Hatched line corresponds to the continuum produced with a
975 second-order polynomial. For the sake of clarity, the residuals (observed – modeled quantity) are shifted
976 by +0.1 which means that a perfect fit, with a zero residual value all along the spectral domain, is
977 displayed with a flat line with a 0.1 ordinate. Two solutions are retained. Fig. 6a. 'OPX' configuration
978 (rms = 0.014). Fig. 6b. 'OL-OPX' configuration (rms=0.006 and the residuals line is clearly smoother
979 along the spectrum). The 'OL-OPX' configuration delivers the best modeling.

980

981 Fig. 7

982 Example of results (same display as fig. 6) given by our approach in the case of the olivine configuration,
983 for three different chemical compositions in the solid solution (respectively $Fo_{0,1}$ (RELAB C1PO58 < 45
984 μm), $Fo_{50,5}$ (RELAB C1PO49 < 45 μm) and $Fo_{96,9}$ (RELAB C1PO52 < 45 μm). Each time the Gaussian
985 functions parameters are in agreement with literature trends.

986

987 Fig. 8

988 Effect of olivine grains size on the spectral shape (left) and corresponding MGM results (right). Olivine
989 (Hawaii) has a fixed chemical composition (forsterite Fo_{88}). Spectra have been measured with an ASD
990 FieldSpec[®] at our laboratory (DTP/UMR 5562). Large grains size forsterite displays absorption
991 characteristics that may mimic fayalite absorption features. This effect, not really documented in the
992 literature appears when the grains size exceeds 250 μm .

993

994 Fig. 9

995 Example of results (same display as fig. 6) given by our approach in the case of spectra of various
996 pyroxenes showing different chemical compositions. Gaussians are displayed with a hatched-dotted black
997 line for clinopyroxene and a solid black line for orthopyroxene. Solid grey line corresponds to Gaussian
998 "1200". Hatched line corresponds to the continuum produced with a second-order polynomial. Fig. 9a:
999 case of synthetic pyroxenes (Klima et al., 2007): (1) refers to Enstatite ($En_{97}Fs_2$) (RELAB C1DL64A), (2)
1000 refers to Ferrosilite (En_0Fs_{100}) endmember (RELAB C1DL61A). Fig. 9b: case of natural pyroxenes
1001 (pigeonite $Wo_8En_{65}Fs_{27}$ (RELAB C1PP42) and augite $Wo_{39}En_{42}Fs_{19}$ (RELAB C1PP49)). Orthopyroxene
1002 configuration is kept in the case of enstatite, ferrosilite and pigeonite while clinopyroxene configuration is
1003 kept for augite. Gaussian functions parameters are in agreement with literature trends.

1004

1005 Fig. 10

1006 Evolution of MGM calculated centers at 1 and 2 μm compared to pyroxenes trend defined by Adams
 1007 (1974). Left (Fig. 10a): in the case of a synthetic orthopyroxene set (Klima et al., 2007) ranging from
 1008 enstatite ($\text{En}_0\text{Fs}_{100}$) to ferrosilite ($\text{En}_{97}\text{Fs}_2$). Right (Fig. 10b): examples of various pyroxenes coming from
 1009 the RELAB library (compositions are respectively: (1) diopside $\text{Wo}_{49}\text{En}_{43}\text{Fs}_8$ (C1PP29), (2) diopside
 1010 $\text{Wo}_{45}\text{En}_{45}\text{Fs}_{10}$ (C5PP21), (3) enstatite $\text{Wo}_1\text{En}_{91}\text{Fs}_8$, (C1PP43), (4) enstatite $\text{Wo}_1\text{En}_{87}\text{Fs}_{12}$, (C5PE30), (5)
 1011 pigeonite $\text{Wo}_8\text{En}_{65}\text{Fs}_{27}$ (C1PP42) and (6) augite $\text{Wo}_{39}\text{En}_{42}\text{Fs}_{19}$ (C1PP49),). Error bars correspond to
 1012 uncertainties from Kanner et al. (2007), i.e. ± 8 nm in the 1 μm domain and ± 17 nm in the 2 μm domain.
 1013 Pyroxenes 2 and 4, are the two pyroxene endmembers used in the case of diopside/enstatite mixtures from
 1014 Sunshine and Pieters (1993). The present MGM results agree with Adams (1974) except for the case of
 1015 pigeonite which appears slightly off trend.

1016

1017 Fig. 11

1018 Chemical compositions estimated from Gaussian centers parameters. Left: data from Hazen et al. (1978);
 1019 Right: data from Cloutis and Gaffey (1991). Pyroxenes used are those described in Figure 10. In the four
 1020 quadrilaterals, each circle indicates the true chemical composition of the corresponding pyroxene (data
 1021 from RELAB). Colors within the circles and in the background correspond respectively to the absorption
 1022 center position at 1 and 2 μm obtained by our approach, and to the determinations found by Hazen et al.
 1023 and Cloutis and Gaffey. That way, if the MGM result is in agreement with literature data, the color inside
 1024 the circle must be the same as the surrounding background color,

1025

1026 Fig. 12

1027 MGM calculated centers at 1 and 2 μm compared to pyroxenes trend defined by Adams (1974) in the case
 1028 of diopside/enstatite mixture (<45 μm micron particles suite) from Sunshine and Pieters (1993). The two
 1029 minerals have a fixed chemical composition and only their relative abundance varies (i.e. Gaussian
 1030 centers should be always the same as 2 and 4 in Fig. 9). Bold crosses correspond to the center band
 1031 positions found with MGM deconvolution by Sunshine and Pieters (1993) for the pyroxene end-member
 1032 spectrum (respectively, 0.91, 1.83 μm for opx, and 1.01, 2.27 μm for cpx mineral. Symbols (cross,
 1033 triangle, losange) indicate the MGM configuration used in the present approach, respectively 'OPX',
 1034 'CPX', 'CPX-OPX'. Figures mentioned within the symbols indicate the proportion of clinopyroxene in the
 1035 mixture. Concerning the opx detection, one notes that for both 'OPX' and 'CPX-OPX' configurations the
 1036 result for the opx 1 μm band center positions is extremely stable whatever the mixture while a progressive
 1037 shift is seen for the opx 2 μm band center position when the cpx mineral prevails in the mixture (60, 75,
 1038 85%). Concerning the cpx detection, for both 'CPX' and 'CPX-OPX' configurations, the 1 μm band
 1039 center position is well determined whatever the mixture while some scattering on the order of 30-40 nm is
 1040 observed with the 2 μm band center position. For high cpx proportions (75, 85, 100%),
 1041 the 'CPX' configuration returns very close solutions (within 10 nm) compared to the reference case.

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1043

1044 Fig. 13

1045 Band center position of orthopyroxene Gaussians at 1 and 2 μm and olivine Gaussians at 0.85, 1.05 and
 1046 1.2 μm from MGM deconvolution for olivine-pyroxene(s) mixtures spectra. A set of spectra with binary
 1047 mixtures of olivine (Fo_{90}) (referred to as endmember Fo_1) and low-calcium pyroxene (hypersthene)
 1048 (referred to as endmember En_1) ranging from (10%Ol, 90%LCP) to (90%Ol, 10%LCP) (referred to as
 1049 C1AG14, and C1AG17 to C1AG20 in the RELAB collection) has been used first. MGM results are
 1050 displayed by means of losange symbol.

1051 Then, a dedicated set of spectra with different amount of olivine (Fo_{85-89}) (referred to as endmember Fo_2),
 1052 orthopyroxene (En_{85-90}) (referred to as endmember En_2) and plagioclase ($\text{An}_{78}\text{Ab}_{22}$) has also been
 1053 analyzed. MGM results are displayed by means of triangle symbol. Open symbols (losange and triangle)
 1054 refer to the use of monomineral configurations, either 'OPX' or 'OL' one. Filled symbols (grey-colored
 1055 losange and triangle) refer to the use of 'OL-OPX' configuration. Cross symbol refers to the 'OL-OPX-
 1056 CPX' configuration applied to the spectra with a ternary mixture (ol,opx,cpx) (see also figure 14). Large
 1057 scale symbols on the 0% vertical axis represent the orthopyroxene bands center for En_1 and En_2
 1058 endmembers; shaded large scale symbols on the 100% vertical axis represent the olivine bands center for
 1059 Fo_1 and Fo_2 endmembers. Small size triangles correspond to En_1 mixed with variable plagioclase
 1060 proportions: results demonstrate the orthopyroxene band center positions are unaffected

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1062 Fig. 14

1063 MGM deconvolution (same display as Fig. 6) for the case of a ternary mafic mixture (20% ol, 20% opx,
 1064 60% cpx) spectrum from RELAB (C1XS03). Gaussians are displayed with a hatched-dotted black line for
 1065 clinopyroxene, a solid black line for orthopyroxene and a dotted grey line for olivine. Solid grey lines
 1066 correspond to Gaussians "650" and "1200". Hatched line corresponds to the continuum produced with a
 1067 second-order polynomial. Fig. 14A: 'CPX' configuration, Fig. 14B: 'CPX-OPX' configuration, Fig. 14C:
 1068 'CPX-OL' configuration, Fig. 14D: 'CPX-OPX-OL' configuration. The band center position for olivine
 1069 and orthopyroxene Gaussians are displayed with crosses on figure 13 (see Fig. 13).

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1071 Fig. 15

1072 MGM analysis of a ternary mafic mixture (20% ol, 20 % opx, 60% cpx) spectrum. Orthopyroxene and
 1073 clinopyroxene band center positions determined by MGM deconvolution plotted over Adams (1974)
 1074 representation. Symbols (triangle, star, losange, square) indicate the successive MGM configurations used
 1075 in the present approach, respectively 'CPX', 'OL-CPX', 'OPX-CPX', 'OL-OPX-CPX'. Their size reflects
 1076 the MGM associated uncertainty (on the order of 10-20 nm) on a band center position (Kanner et al.,
 1077 2007). Letters A, B, C refer to the three spectra used (see text and table 5 for details). Results with A, B,
 1078 C spectra appear very consistent for each configuration. Clinopyroxene mineral which is dominant is
 1079 correctly determined with the 'CPX' configuration, in close agreement with the results returned by the
 1080 'OL-CPX' configuration. Then, orthopyroxene mineral is consistently detected by both the 'OPX-CPX'
 1081 and 'OL-OPX-CPX' configurations. While the results for the cpx 1 μm band and the opx 2 μm band

1082 center positions are quite stable whatever the configuration, the opx 1 μm band and the cpx 2 μm band
1083 center positions shift by a few tens of nanometers and are responsible for the observed scattering, which
1084 however does not hamper the detection of the three mafic minerals.

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1088 **Table 1**

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	OL	OPX	CPX	OL-OPX	OL-CPX	OPX-CPX	OL-OPX-CPX
450	X	X	X	X	X	X	X
650		X	X	X	X	X	X
850	X			X	X		X
900		X		X		X	X
1000			X		X	X	X
1050	X			X	X		X
1200		X	X			X	
1250	X			X	X		X
1800		X		X		X	X
2150			X		X	X	X
Tot. Nb.	4	5	5	7	7	7	9

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1092 **Table 2**

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Relab spectrum	Fo	Grain size	<i>rms</i>
C1PO58	0,1	< 45 μm	0,0040
C3PO59	0,1	45 - 90 μm	0,0070
C1PO48	27,7	< 45 μm	0,0094
C1PO72	36,0	< 45 μm	0,0041
C1PO74	42,0	< 45 μm	0,0038
C1PO49	50,5	< 45 μm	0,0055
C1PO47	59,3	< 45 μm	0,0099
C1PO45	60,0	< 45 μm	0,0098
C1PO30	82,4	< 45 μm	0,0046
C2PO31	82,4	< 45 μm	0,0024
C1OL01	85,0	< 45 μm	0,0044
C2OL08	85,7	< 45 μm	0,0064
C1PO64	85,9	< 45 μm	0,0049
C1PO40	88,0	< 45 μm	0,0049
C3PO57	88,5	> 45 μm	0,0088
C1PO27	89,0	< 45 μm	0,0057
C1OL02	90,0	< 45 μm	0,0068
CAPO50	90,4	< 45 μm	0,0024
C2OL04	90,5	< 45 μm	0,0026
C2OL10	90,8	< 45 μm	0,0052
C1OL03	91,0	< 45 μm	0,0132
C1PO60	91,8	< 45 μm	0,0041
C3PO61	91,8	> 45 μm	0,0067
C1PO76	92,0	< 45 μm	0,0030
C1PO77	92,0	> 45 μm	0,0035
C3PO54	92,7	> 45 μm	0,0406
C1PO52	96,9	< 45 μm	0,0026
C3PO53	96,9	> 45 μm	0,0035

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1096 **Table 3**

Relab spectrum	Mixture composition		Configuration kept (rms)		
	Opx	Cpx	OPX	OPX-CPX	CPX
C5PE30	100%	0%	0.0041		
C1XP15	85%	15%	0.0039	0.0036	
C1XP13	75%	25%	0.0045	0.0035	
C1XP11	60%	40%	0.0054	0.0031	
C1XP10	50%	50%		0.0027	
C1XP12	40%	60%		0.0027	
C1XP14	25%	75%		0.0027	0.0096
C1XP16	15%	85%		0.0030	0.0083
C5PP21	0%	100%			0.0050

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1122 **Table 4**

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Relab spectrum	Mixture composition			Relative proportion		Configuration kept (rms)		
	OI	Opx	PI	OI	Opx	OL	OPX	OL-OPX
CCPA60	0%	0%	100%	0%	0%			
C3PE41	0%	100%	0%	0%	100%		0.0185	
C1XT29	0%	75%	25%	0%	100%		0.0148	
C1XT28	0%	50%	50%	0%	100%		0.0132	
C1XT27	0%	25%	75%	0%	100%		0.0131	
CCPO81	100%	0%	0%	100%	0%	0.0065		
C1XT24	75%	0%	25%	100%	0%	0.0144		
C1XT25	50%	0%	50%	100%	0%	0.0213		
C1XT26	25%	0%	75%	100%	0%	0.0278		
C1XT34	17%	67%	17%	20%	80%		0.0130	
C1XT30	25%	75%	0%	25%	75%		0.0152	
C1XT37	17%	42%	42%	29%	71%		0.0118	
C1XT31	50%	50%	0%	50%	50%		0.0147	0.0064
C1XT39	42%	42%	17%	50%	50%		0.0139	0.0051
C1XT36	33%	33%	33%	50%	50%		0.0127	0.0053
C1XT35	17%	17%	67%	50%	50%		0.0131	0.0103
C1XT38	42%	17%	42%	71%	29%		0.0125	0.0080
C1XT32	75%	25%	0%	75%	25%			0.0049
C1XT33	67%	17%	17%	80%	20%			0.0057
C1AG09	0%	100%	0%	0%	100%		0.0104	
C1AG17	10%	90%	0%	10%	90%		0.0080	0.0042
C1AG18	30%	70%	0%	30%	70%		0.0079	0.0039
C1AG19	50%	50%	0%	50%	50%		0.0074	0.0024
C1AG14	70%	30%	0%	70%	30%		0.0083	0.0023
C1AG20	90%	10%	0%	90%	10%			0.0023
C1AG08	100%	0%	0%	100%	0%	0.0036		

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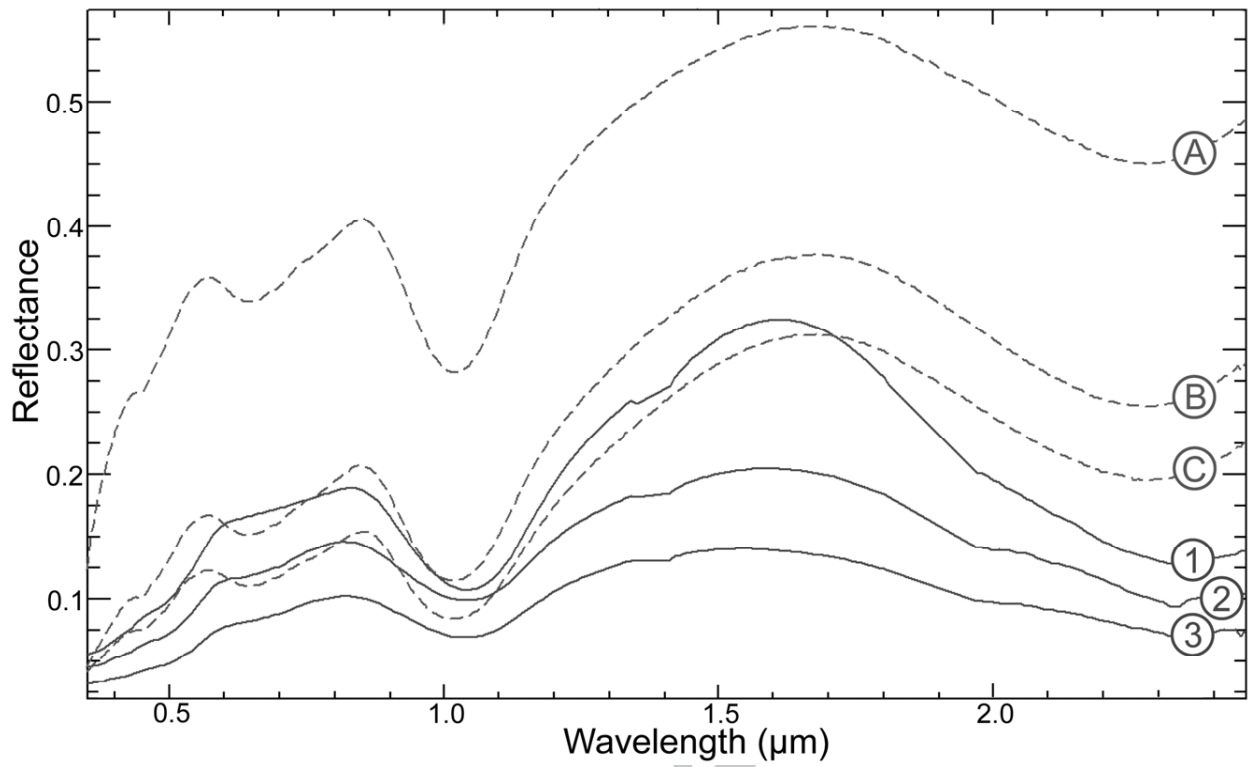
Table 5

Relab spectrum	Grain size			Configuration kept (rms)			
	Cpx	Opx	OI	CPX	OL-CPX	OPX-CPX	OL-CPX-OPX
C1XS01 (A)	MS	MS	MS	0.0065	0.0065	0.0026	0.0024
C1XS03 (B)	LS	LS	SS	0.0050	0.0047	0.0028	0.0025
C1XS02 (C)	SS	SS	LS	0.0060	0.0056	0.0026	0.0026

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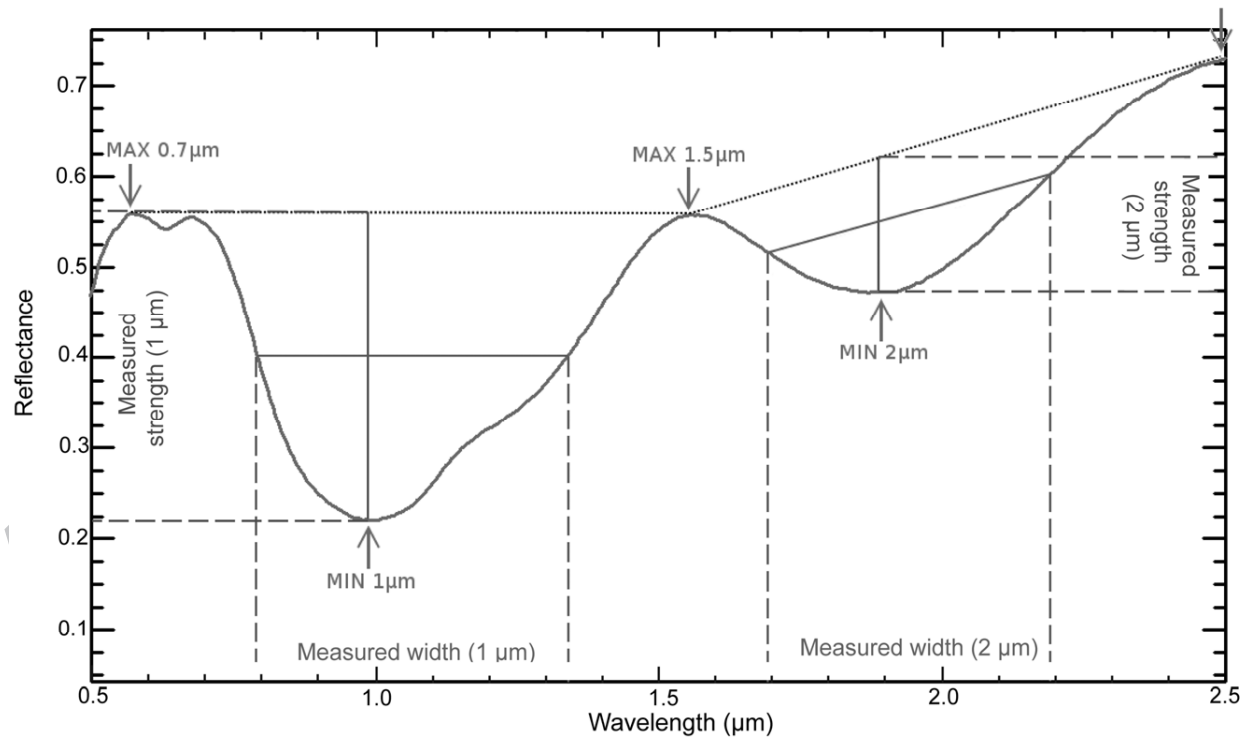
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1133 **Figure 1**

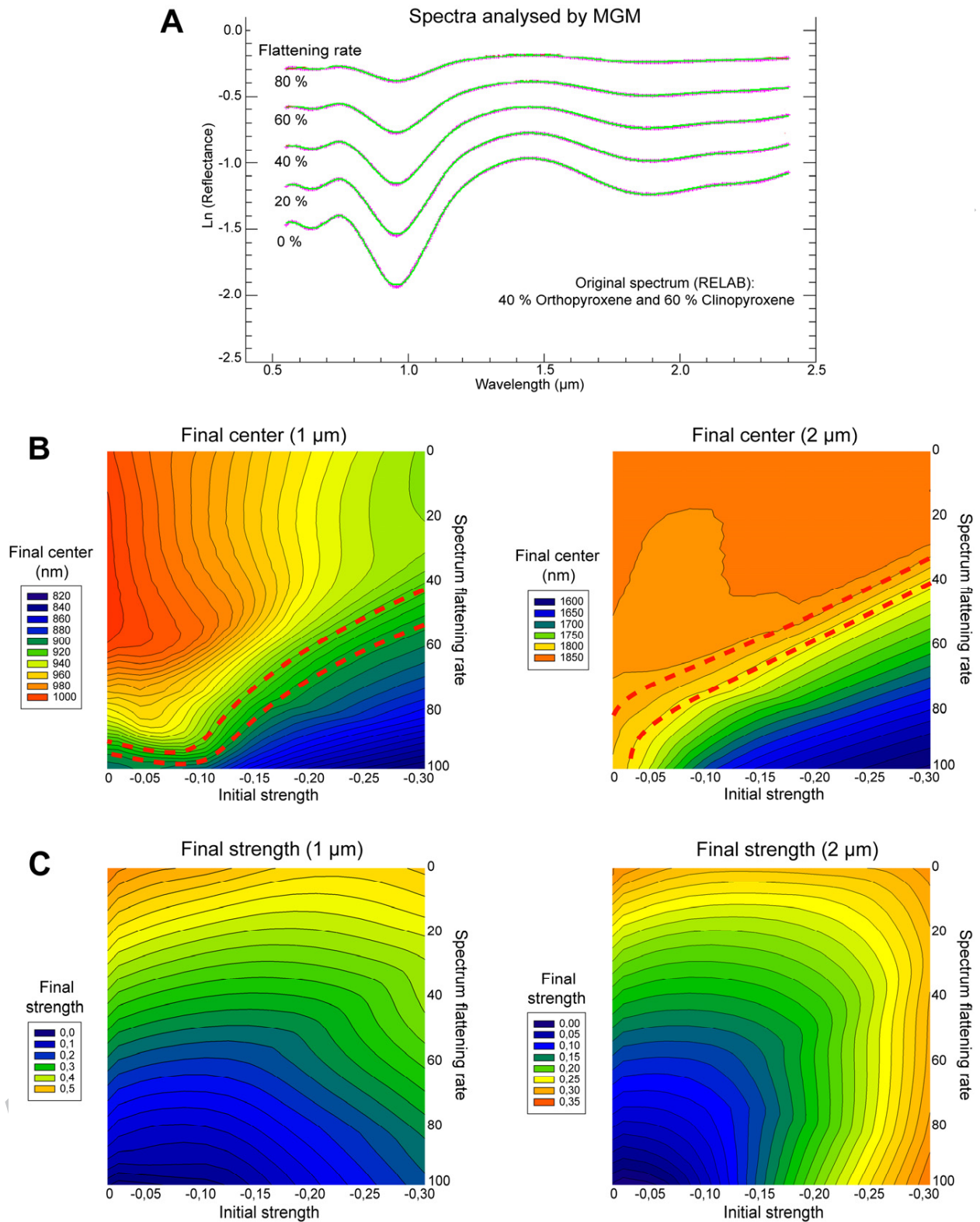
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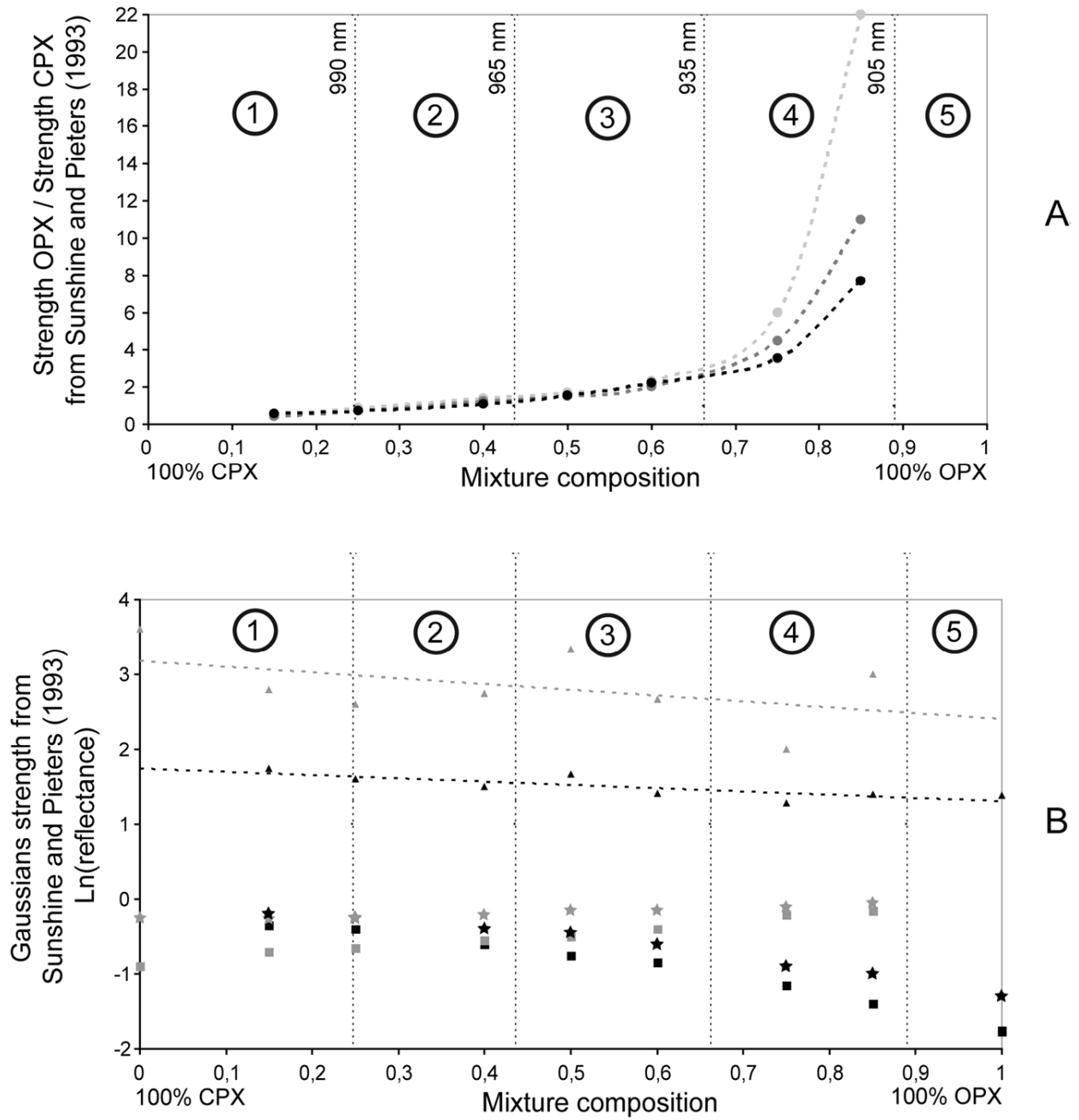
1136 **Figure 2**

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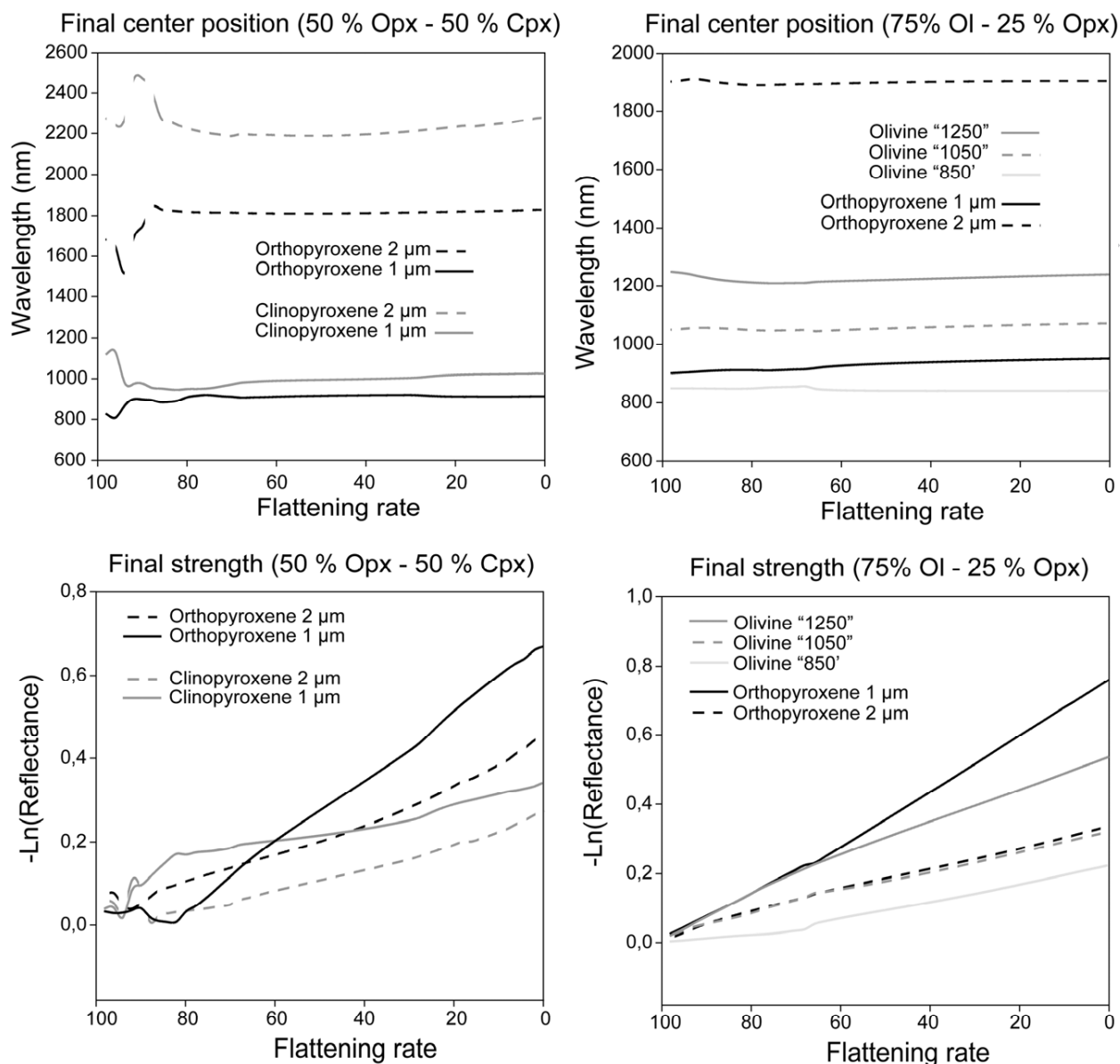
1139 **Figure 3**



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Figure 4

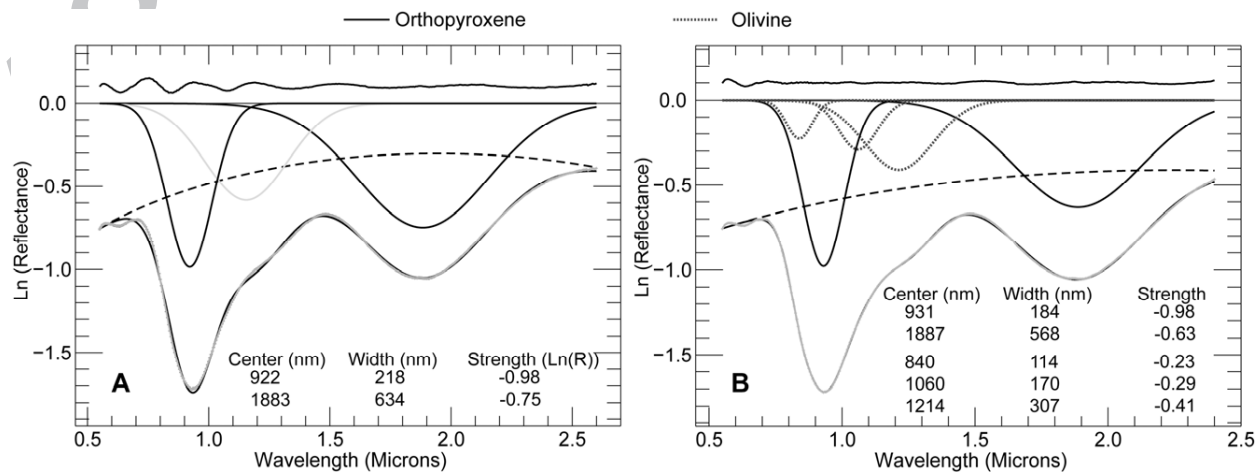


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1143 **Figure 5**

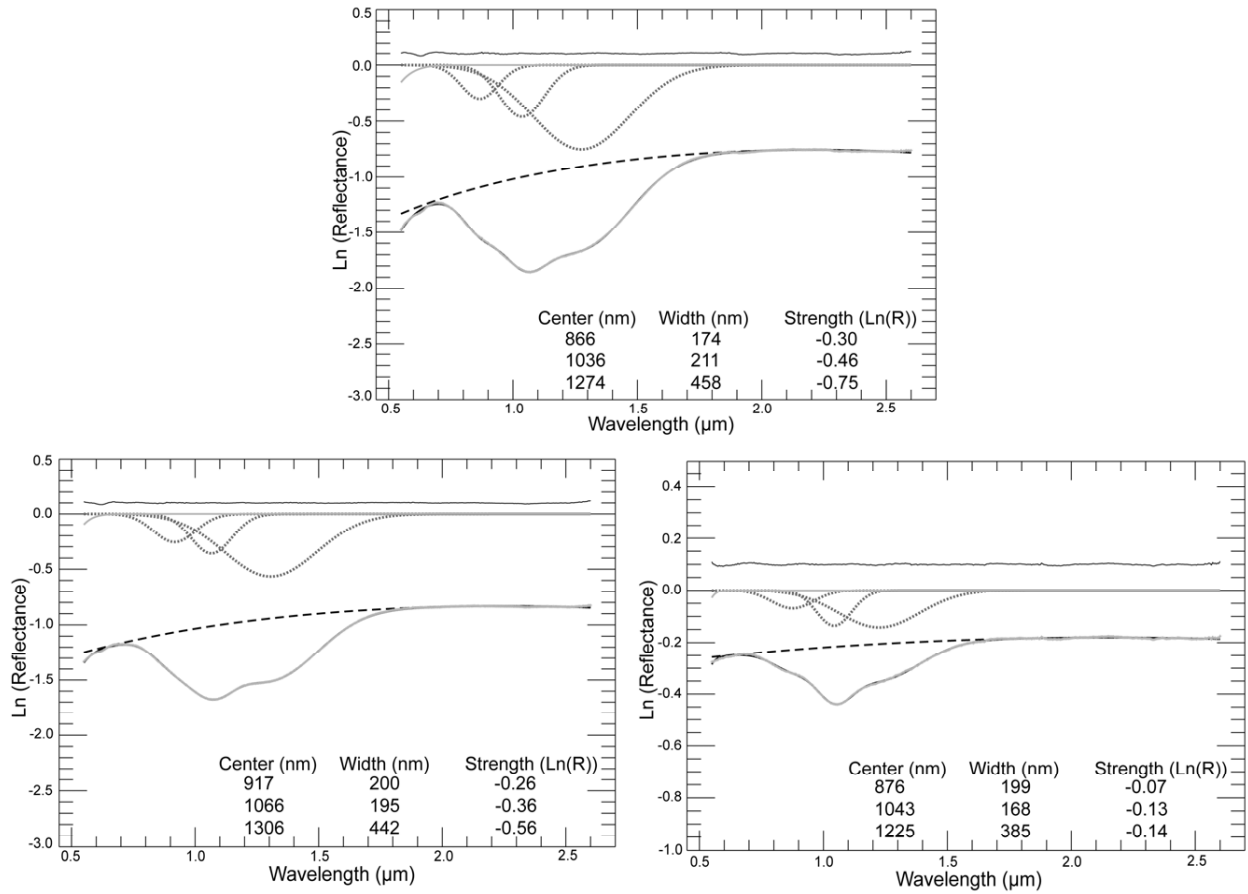
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1147 **Figure 6**



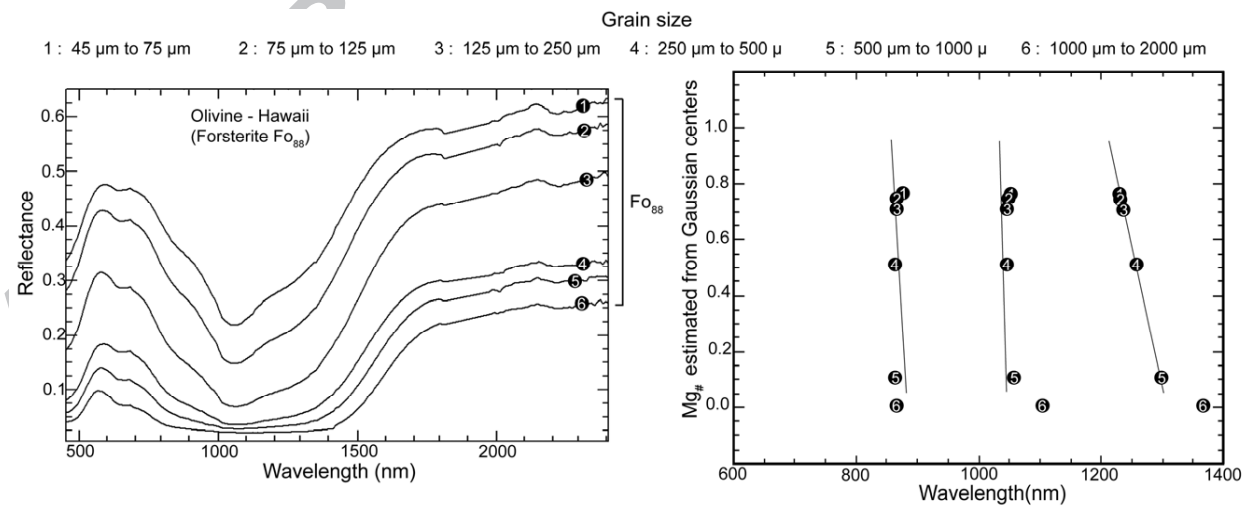
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1149 **Figure 7**

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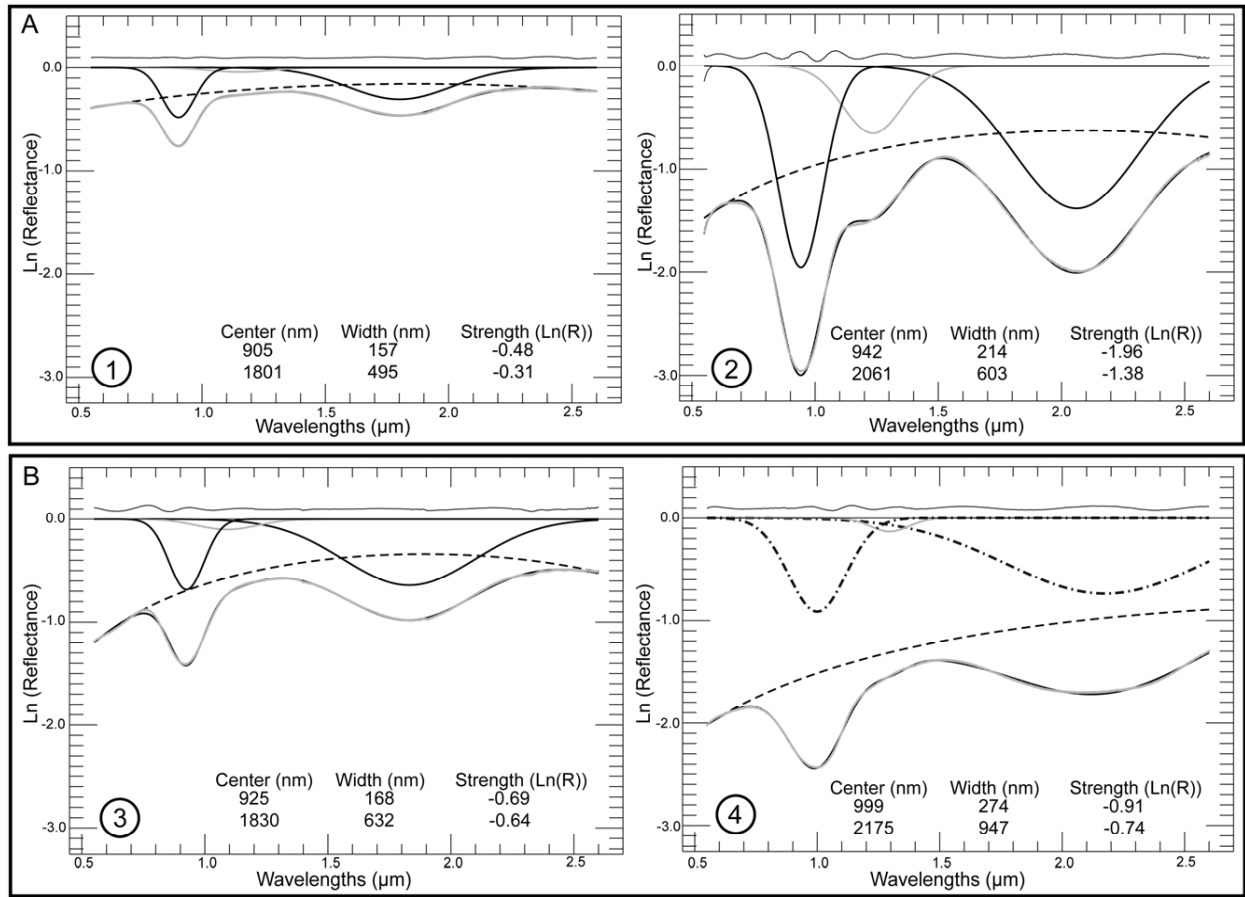
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1154 **Figure 8**



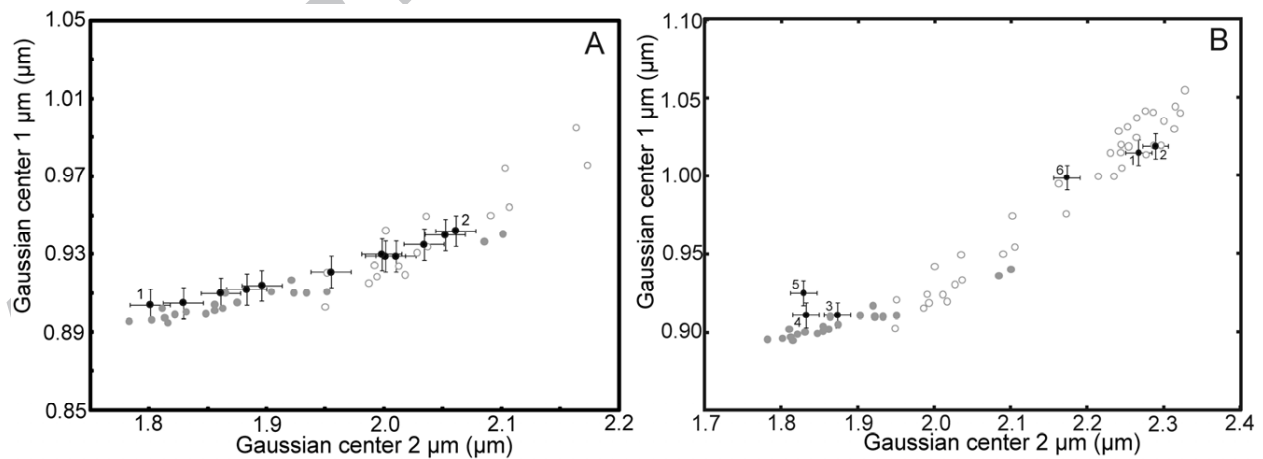
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1156 **Figure 9**

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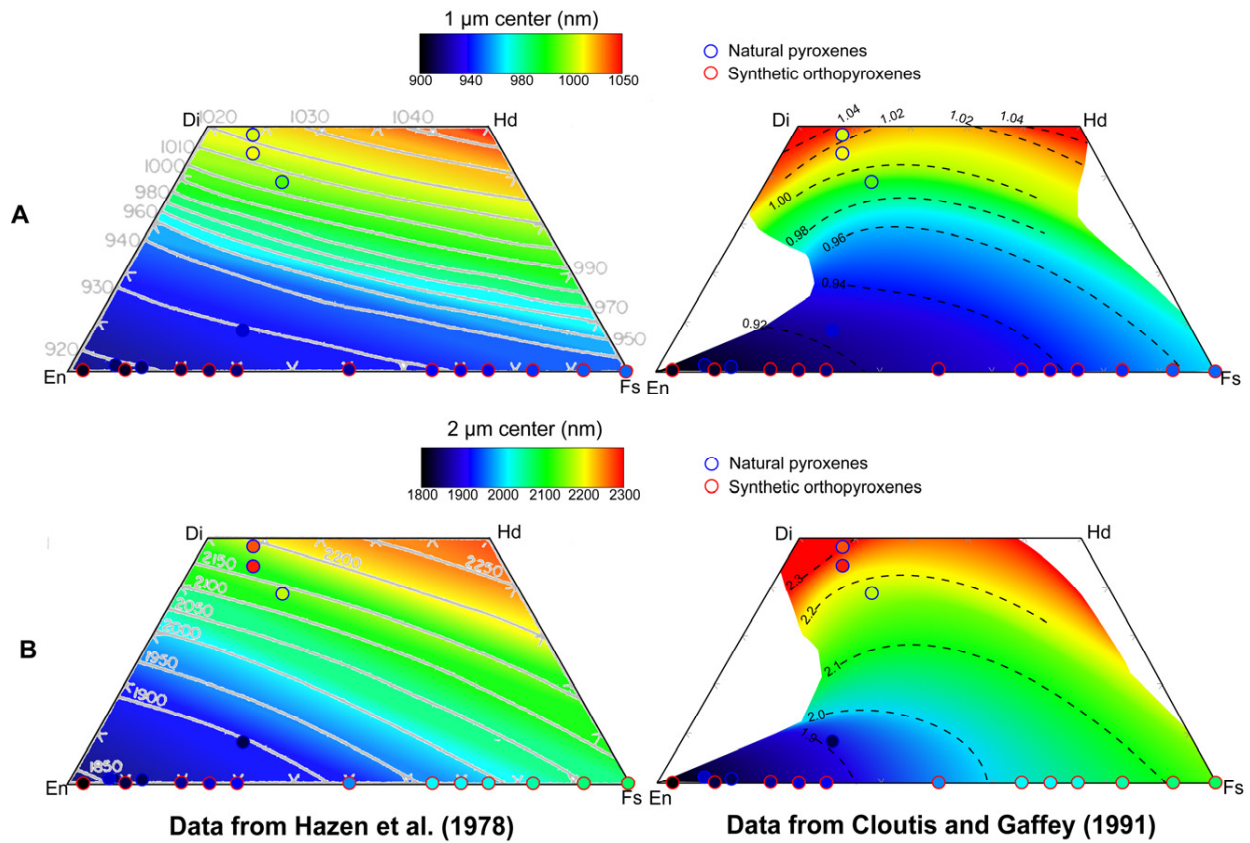
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1161 **Figure 10**

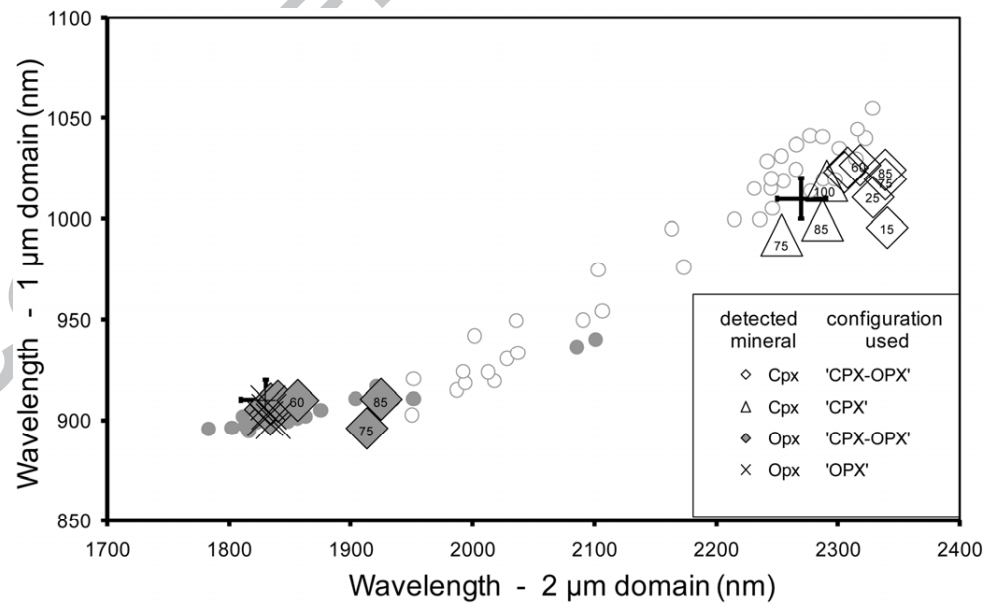


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1163 **Figure 11**

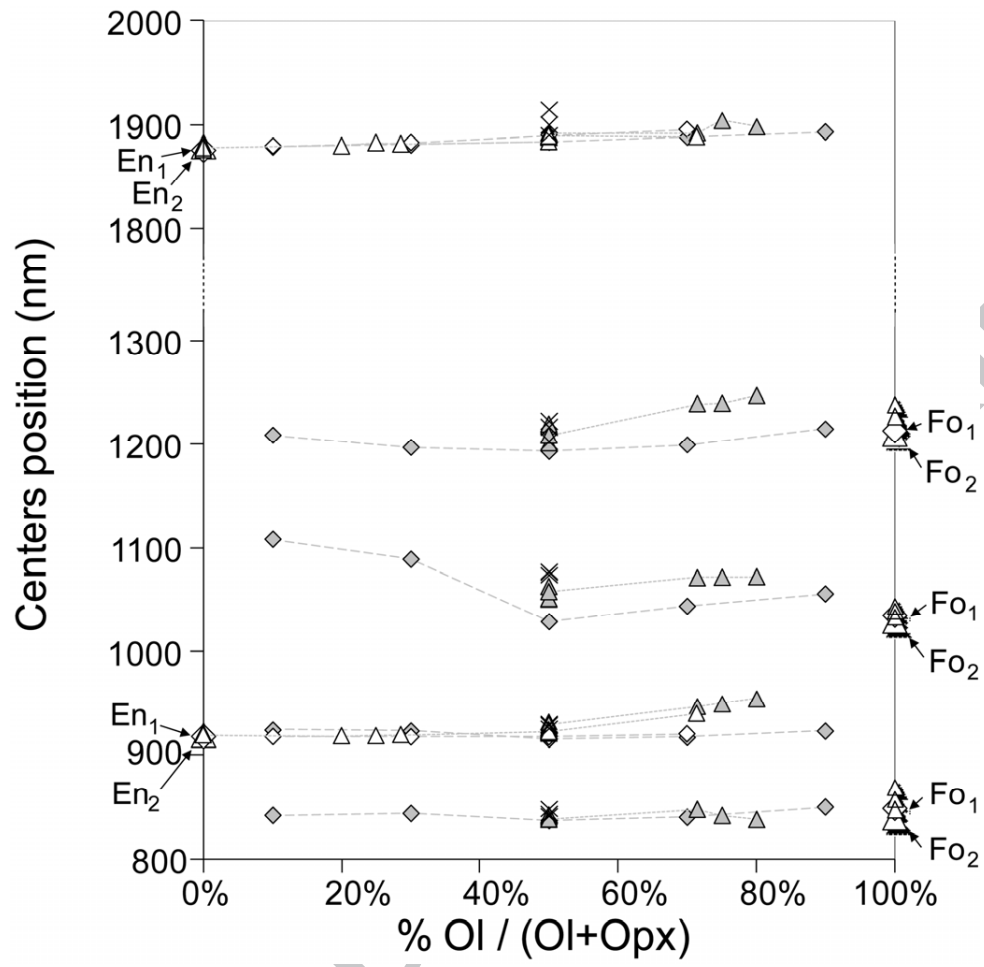
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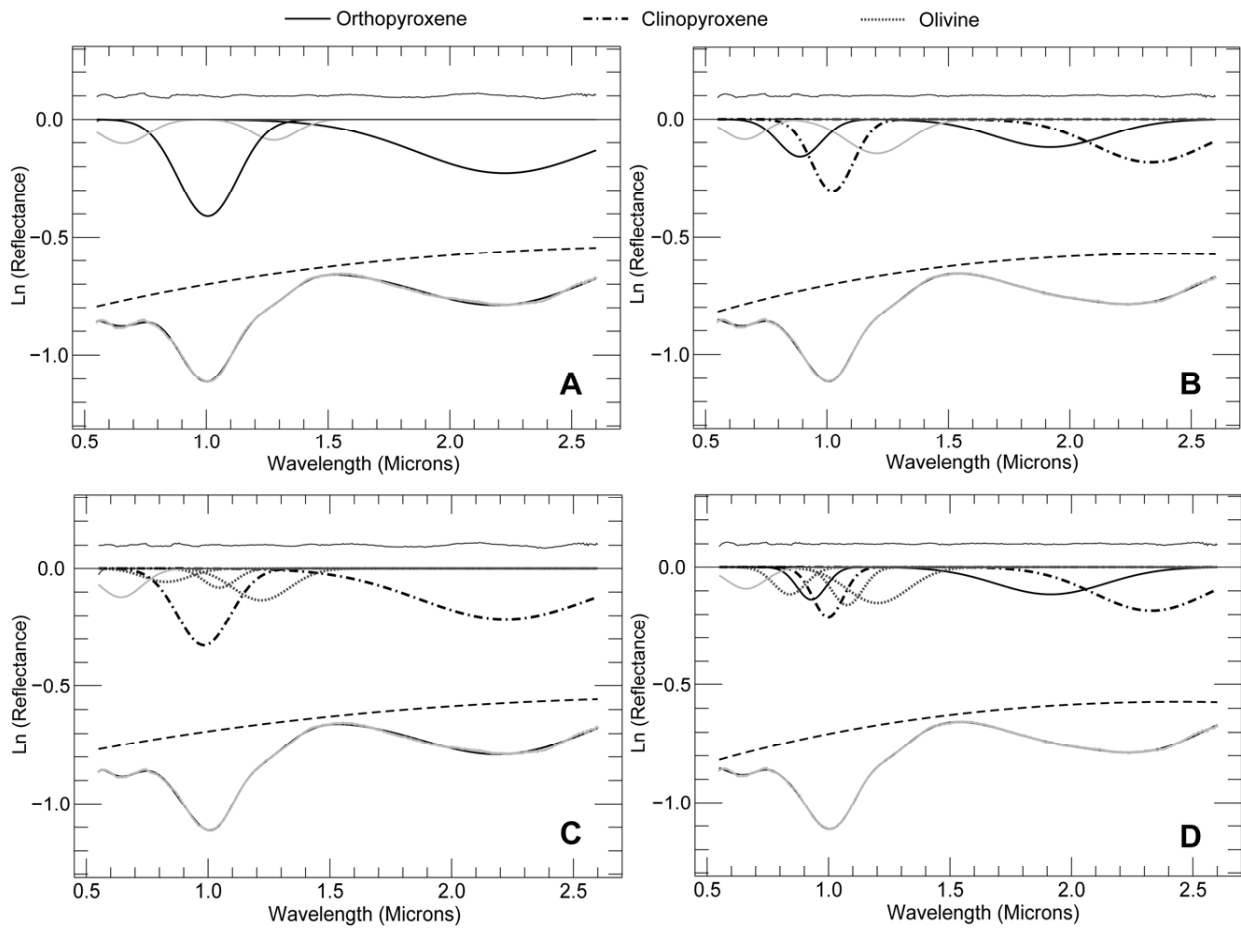
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1167 **Figure 12**



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1169 **Figure 13**



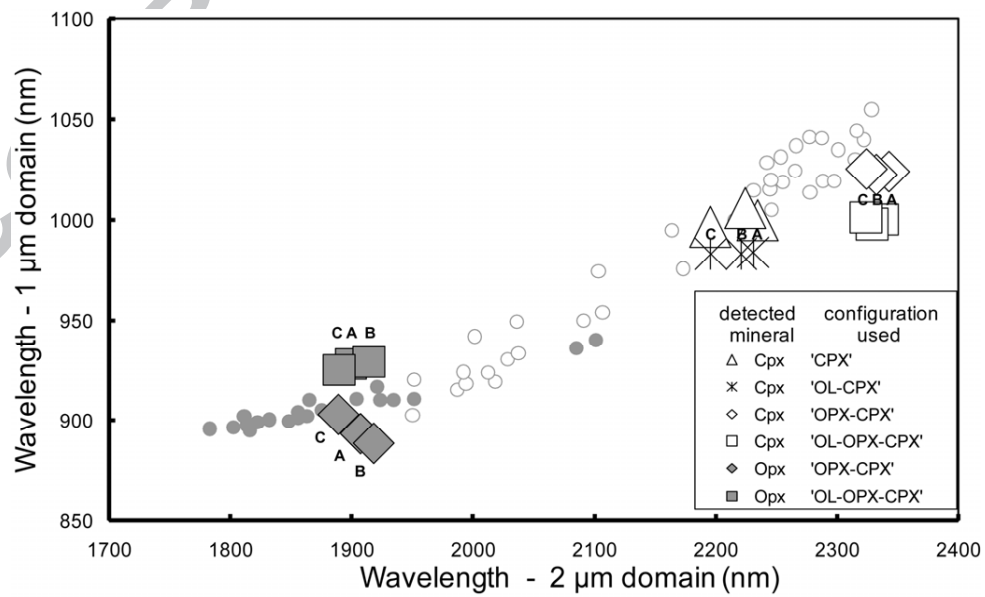
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1171 **Figure 14**

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1176 **Figure 15**

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1180 > Automatic procedure implemented on the original MGM approach

1181 > Allow to deal with complex mineralogies involving olivine and/or pyroxene(s)

1182 > Demonstration on binary and ternary mixtures with different chemical compositions

1183 > Interpretation of MGM outputs in terms of modal and chemical compositions

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