
Introduction: The CheMin instrument on the Mars Science Laboratory rover Curiosity performed X-ray diffraction analyses on scooped soil at Rocknest [1,2,3] and on drilled rock fines at Yellowknife Bay (John Klein and Cumberland samples) [3,4]. The Kimberley (Windjana sample) [3,5], and Pahrump (Confidence Hills sample) [3,6] in Gale crater, Mars. Samples were analyzed with the Rietveld method to determine the unit-cell parameters and abundance of each observed crystalline phase. Unit-cell parameters were used to estimate compositions of the major crystalline phases using crystal-chemical techniques. These phases include olivine, plagioclase and clinopyroxene minerals. Comparison of the CheMin sample unit-cell parameters with those in the literature provides an estimate of the chemical compositions of the major crystalline phases.

Preliminary unit-cell parameters, abundances and compositions of crystalline phases found in Rocknest and Yellowknife Bay samples were reported in [1,2,4]. Further instrument calibration, development of 2D-to-1D pattern conversion corrections, and refinement of corrected data allows presentation of improved compositions for the above samples.

Composition as a Function of Unit-Cell Parameters: Unit-cell parameters and chemistry were obtained from the literature for the target minerals, and relationships between cell parameters and chemistry were observed. Some relationships, like that of Fa-Fo olivine (fig. 1), are very well defined, whereas others, such as coupled substitution in plagioclase, are not as well defined. In the case of plagioclase, diffraction patterns from these samples have broad peaks and indications from pattern fitting are that more than one plagioclase phase or zoned plagioclase may be present. Work is ongoing in addressing plagioclase compositions, but at present the use of cell parameters in constraining plagioclase composition is limited.

Augite and pigeonite were constrained to the Ca-Fe-Mg system. A simple binary plot, as shown in Fig. 1, does not fully describe the relationship between composition and cell dimensions. Therefore, in both clinopyroxenes, Mg-content was estimated from the b unit-cell parameter because it forms a linear trend (Fig. 2a). Ca and Fe were discriminated by the β angle for augite (Fig. 2b) and by unit-cell volume for pigeonite (not shown).

Chemical Composition of Olivine and Clinopyroxene Group Minerals: The following chemical compositions were obtained from the regressions illustrated in Fig.1-2:

<table>
<thead>
<tr>
<th></th>
<th>Rocknest</th>
<th>John Klein</th>
<th>Cumberland</th>
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<tbody>
<tr>
<td>olivine</td>
<td>(Mg$<em>{0.81}$Fe$</em>{1.19}$)SiO$_4$</td>
<td>olivine (Mg$<em>{0.98}$Fe$</em>{1.02}$)SiO$_4$</td>
<td>olivine (Mg$<em>{0.76}$Fe$</em>{1.22}$)SiO$_4$</td>
</tr>
<tr>
<td>augite</td>
<td>(Ca$<em>{0.70}$Mg$</em>{0.68}$Fe$_{0.62}$)Si$_2$O$_6$</td>
<td>augite (Ca$<em>{0.48}$Mg$</em>{0.50}$Fe$_{0.49}$)Si$_2$O$_6$</td>
<td>augite (Ca$<em>{0.88}$Mg$</em>{0.66}$Fe$_{0.49}$)Si$_2$O$_6$</td>
</tr>
<tr>
<td>pigeonite</td>
<td>(Mg$<em>{0.97}$Fe$</em>{0.67}$Ca$_{0.36}$)Si$_2$O$_6$</td>
<td>pigeonite (Mg$<em>{1.14}$Fe$</em>{0.71}$Ca$_{0.15}$)Si$_2$O$_6$</td>
<td>pigeonite (Mg$<em>{1.10}$Fe$</em>{0.68}$Ca$_{0.22}$)Si$_2$O$_6$</td>
</tr>
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Figure 1. Mg-content of Fa-Fo olivine as a function of unit-cell volume. Individual points obtained from literature data (shown as blue dots). Unit-cell volumes of Rocknest, John Klein and Cumberland samples are represented by a red diamond, blue square and green triangle, respectively. Estimated Mg-content for each CheMin sample was determined using this regression line.
Figure 2a. Variation of Mg-content with $b$ unit-cell parameter in augite obtained from literature data (individual values shown as blue dots). The estimated Mg-contents of the CheMin samples were determined from this regression. The $b$ unit-cell parameters for the Rocknest, John Klein and Cumberland samples plot closely and are represented by a red diamond, blue square and green triangle, respectively.

Figure 2b. Ca-content in augite is obtained by scaling the separation between the two trends of individual literature values of Mg-content versus $\beta$ angle at Ca = 1 apfu (dashes) and Ca = 0.8 apfu (circles). The Mg-content from fig. 2a at the refined $\beta$ angles of the Rocknest, John Klein and Cumberland samples are represented by a red diamond, blue square and green triangle, respectively.

Comparison with Bulk Chemistry Measured by APXS: The Martian samples analyzed by CheMin, like many terrestrial sediments and sedimentary rocks, contain both amorphous and crystalline components. The bulk crystalline chemistry was computed from the combination of the estimated chemical compositions of the major phases and the ideal compositions of the minor phases, each weighted by their respective abundances. The amorphous component composition is computed using the following matrix equation. We assume the crystalline component, C, plus the “amorphous” component, A, sum to the total measured by the Alpha-Particle X-ray Spectrometer (APXS), T, where $\alpha$ is a scaling factor:

$$\alpha C + (1-\alpha)A = T$$

$\alpha$ is the portion of the material that is crystalline, the upper limit of which is used in these calculations. The upper limit was chosen because it is the point at which the crystalline component has taken up the entire limiting element from the bulk composition, thereby constraining the maximum possible proportion of crystalline material in the sample. Our results agree with those estimated by [7], where representative phase compositions from martian meteorites were used. This agreement provides a measure of consistency between reported chemistry of Martian meteorites and CheMin results.