Improving the accuracy of unitcell parameters obtained from the CheMin instrument on Mars through an internally calibrated sample cell offset

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X-ray CheMin diffraction onboard the Mars Science Laboratory rover Curiosity is equipped with 5 sealed calibration standards and 27 reusable sample cells [1]. Sediment and drilled rock fines from the Martian surface are delivered to reusable sample cells for analysis by X-ray diffraction. The diffraction patterns are returned to Earth where unit-cell parameters of major phases are determined with the Rietveld refinement method. In some cases, the comparative systematics of the refined unit-cell parameters do not align with those observed from terrestrial diffractometers. The cause for this discrepancy is sample offset up to 50 microns from the ideal diffracting position, related machining of the sample cells. Varying an offset parameter during pattern processing has the effect of varying refined cell parameters. Consequently, the offset parameter can be calculated based on unit-cell parameter deviation from terrestrial Plagioclase is present in all of the CheMin samples and is thus used to calculate the sample cell offset, improving the accuracy of unit-cell parameter refinements for all major phases.

[1] Blake et al. (2012) Space Sci Rev, **170**, No. 1-4, 341-399