# Supporting Information for

# Mineralogy of the Windjana Sandstone (Kimberley Area, Gale Crater, Mars) by CheMin X-ray Diffraction: Sediment Components, and the Nature of Potassic Rocks and Sediments in Gale Crater

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# Text S2: Description of Calculation of the Chemical Composition of the Amorphous & Poorly Crystalline Components.

# Text S1: Conversion from 2D diffraction images to 1D conventional diffractograms. By T. Bristow, NASA Ames.

Sixty 2D diffraction images returned from Curiosity, representing 30 hours of analysis of the Windjana sample in cell 13A, were summed using the image processing software ImageJ. ‘Hot’ pixels and abnormally intense spots on the summed 2D pattern, caused by aberrations on the instrument CCD detector and limited granular motion in the sample cell, were removed from the summed image by setting pixel values to those of adjacent pixels. For the purposes of phase identification, quantification and determination of unit cell parameters the processed 2D diffraction pattern was converted into a 1D XRD pattern using GSE\_ADA version 1.09. This is a custom 2D-to-1D conversion program written by Przemek Dera, University of Hawaii. The conversion calculation uses several parameters describing the geometry and specifications of the CheMin instrument. The parameters and values used to calculate the 1D Windjana pattern are:

CCD pixel size = 0.04 x 0.04 mm

Sample to CCD distance = 18.502 mm

X-ray wavelength = 17.906 nm

Position direct beam would hit the detector = 296.929, 6.71501 (x, y)

Tilt of detector away from orthogonal = - 0.186080, -0.206195 (y, z)

Conversion parameter values were optimized using diffraction patterns obtained from the beryl/quartz, arcanite and amphibole standards onboard CheMin while on the martian surface. No scaling or Lorenz corrections were performed during the conversion. In addition, the ‘Dera’ solid angle normalization setting was used.

# Text S2: Description of Calculation of the Chemical Composition of the Amorphous & Poorly Crystalline Components.

The Windjana sample consists of 75% crystalline phases detected as such by CheMin, and 25% amorphous and poorly crystalline material, detected by CheMin as broad humps or bands in the diffraction pattern (main text, Fig. 4). The composition of this chemical component (amorphous & poorly crystalline) was calculated from the APXS chemical composition of the analyzed sample (the Windjana Dump Pile; main text Fig. 3d, Table 3) by subtracting from it the bulk composition of the crystalline material. Because all of the mineral proportions and mineral chemical compositions have associated analytical uncertainties, their uncertainties must be propagated through the calculation to derive realistic uncertainties on the compositions of both the crystalline material and the poorly crystalline material.

Calculations of these compositions and their uncertainties were done in the EXCEL spreadsheet 2015JE004932R-SupportingInformation-ds4.xlsm; first, the chemical composition of each crystalline was calculated from the compositions of its endmembers (e.g., Mg2SiO4 and Fe2SiO4 in olivine) and the molar proportion of those endmembers in the mineral analyzed by CheMin (e.g., olivine of Fo60) – these calculations are on the sheet named ‘Endmembers.’ The values in the ‘Endmembers’ sheet are in Table 2 of the main text, based on data in the spreadsheet Supporting Information 2 here (2015JE004932R-SupportingInformation-ds2.xlsx). Those mineral composition was scaled by their proportions in the crystalline mass of Windjana and added together to give the overall composition of the crystalline material in Windjana. That composition is then scaled by its proportion in the whole Windjana sample, and subtracted from the bulk APXS analysis to give the composition of the remaining material – the amorphous and poorly crystalline substances.

There are significant analytical uncertainties on the bulk Windjana composition, the compositions of each crystalline phase, and the proportions of crystalline phases, and these uncertainties are included in the calculation in a Monte Carlo method. We assume that the uncertainties are independent of each other. Estimated or calculated standard deviations are available for each composition and proportion, and those values (1 standard deviation or 1 ) were included in the calculation by allowing each value to vary randomly around its nominal value by that standard deviation. In EXCEL, this was implemented using the NORMCM.INV and RAND() functions: for example, if EXCEL cell E45 holds the nominal value of a parameter, and cell E46 holds the 1 certainty on that value, multiple calculations of ‘=(E45+NORCM.INV(RAND(),0,E46))’ return a series of numbers that have a mean of the value in cell E45 and a standard deviation of the value in cell E46. The RAND() function in EXCEL returns a pseudo-random number rather than a true random, but the difference is not significant here. Calculations like this are implemented for every mineral composition and mineral proportion, and the bulk composition from APXS, in the sheet “CalculationSheet” of 2015JE004932R-SupportingInformation-ds4.xlsm.

For the Monte Carlo propagation of these analytical uncertainties, a VBA script was implemented to repeatedly apply successive random sets of uncertainties as described above. The user inputs the number of calculations to be done (<5000); the results here are for 2500 such calculations. After each such calculation, its results are copied calculated the “Results” sheet of 2015JE004932R-SupportingInformation-ds4.xlsm. At the end of the multiple calculations, the “Results” sheet calculates averages of all the calculated compositions, and standard deviations for each in row and column forms. These values are reported in the main text, Table 3.