

Spectral Science Test Data

The SAWG prepared a report on their analysis of the test spectra, and an evaluation team from the CMWG assessed the SAWG results.



14 December 2015

From: Mission Sample Scientist (MSS), Harold C. Connolly Jr.

To: Science Executive Council

Subject: Spectral Analysis Test Data Report

Please find attached a copy of the CMWG Spectral Analysis Test Data Report along with a copy of the SAWG Blind Test Report (previously submitted by Mission Asteroid Scientist (MAS), Beth Ellen Clark. The CMWG report was submitted on time meeting the contractual obligations as defined in the Phase C/D Charter. Both reports make recommendations for a path forward based on the outcomes of the CMWG 'blind' test.

Mission Asteroid Scientist Beth Ellen Clark and I are in total agreement on the following: (1) Before any recommendations as defined in the CMWG and SAWG reports can be seriously considered by the Project, or before any new decisions are made concerning the risk the Project is carrying for a potential spectral library, a TIM between key CMWG and SAWG personnel is required, (2) We suggest holding the TIM in January or February, with a report to the Project to be filed on the outcomes of the TIM by MSS and MAS, and (3) We suggest a full discussion of all the issues raised by the reports to occur at the next face-to-face Science Executive Council meeting in January, regardless if the TIM has occurred.

MSS and MAS are pleased to make the following point very clear: The CMWG blind test was an important achievement for the mission and it has provided an excellent venue for testing many aspects of mission operations, including communications, spectral analysis, and scientific consensus interpretation.



Spectral Process Test Data Report

Prepared by

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Executive Summary

The CMWG Evaluation team reviewed the SAWG analysis of the visible/near-IR (VNIR) and thermal emission infrared (TIR) spectra obtained from the blind test samples and made the following findings and recommendations:

Findings:

1. Overall the VNIR and TIR analyses correctly resolve the analog samples and meteorite samples into hydrous and anhydrous groups where hydrated or anhydrous minerals are major constituents.
2. VNIR detection of minor phases at the 5% level was mixed. The VNIR results correctly identified the 5% addition of calcite in 4 of 4 samples, but gave a false positive on 1 sample. VNIR analyses detected the 5% addition of phyllosilicates in 2 of 2 samples, but gave 1 false positive. Pyroxene was identified in 3 of 5 samples at the ~10 wt.% level but gave false positives in two other samples. VNIR did not detect the 5% olivine present in the single hydrated analog test sample that contained olivine.
3. VNIR correctly identified organics in the analog samples at the 5% level with only 2 false positives (at the trace level). However, organics were not identified in any of the meteorite samples. No information was gleaned from the TIR data for the detection of organic features.
4. Not surprisingly, transparent minerals and minerals lacking strong, distinctive absorption features in the visible/near-IR were not detected in the VNIR analyses, including: plagioclase, FeNi metal, troilite, and magnetite.
5. In the TIR analyses of the analog samples, olivine and phyllosilicates were consistently identified when they were major constituents of the mixtures, but pyroxene and plagioclase present in the analog samples at the 10 wt.% level went undetected. However, phyllosilicates were not identified in the spectra of the CM chondrites Murchison and ALH 83100.
6. TIR detection of minor phases at the 5% level was unreliable. Magnetite (as “oxide”) was correctly identified in 4 of 5 hydrous analog samples, but false positives were reported in 4 of 5 anhydrous analog samples. TIR analyses correctly indicated calcite in 4 of 4 samples where it was present at the 5 wt.% level, but generated 4 false positives where calcite was absent. Phyllosilicates (at the 5% level) in the anhydrous analogs was detected in 1 of 2 samples, not detected in 1 sample, and a false positive reported in another.

Recommendations:

1. Assess the impacts to other aspects of the mission if the level-2 requirements (detection of key mineral phases at the 5% level) cannot be met. The CMWG evaluation team considers this a distinct possibility given the outcome of the blind test.
2. Update spectral libraries to include fine particulates. Identify key minerals and phases of interest known to be in carbonaceous chondrites that have yet to be measured. Survey existing measurements of fine particulate minerals and phases of interest measured under ambient and simulated asteroid environment (SAE) conditions at ASU and other laboratories.

3. Perform a targeted study on the effects of particle size and mineral chemistry on linear unmixing of fine particulate samples.
4. We recommend that TIR spectra be obtained from the analog organic matter that was prepared for the blind test and then use the data to test the detection of organics in the analog blind test samples.
5. We recommend that the VNIR and TIR analyses should be coordinated so that each benefits from their respective insights. This approach might help to resolve some of the ambiguities in phase detection.
6. We recommend that additional independent measurements of the modal mineralogy of the meteorite samples used in the blind test be obtained through additional analytical means (e.g. point-counting of thin sections in the electron microscope/microprobe, μ -FTIR reflectance measurements, etc.).
7. Perform a literature review on the spectral effects of space weathering on organics and other key phases in carbonaceous chondrites. The literature survey should identify key knowledge gaps and suggest targeted experiments to address those gaps.

Introduction

The CMWG is responsible for the analysis of carbonaceous meteorite samples that are analogous to the regolith expected on the surface of Bennu. It is the responsibility of the CMWG to define the sample set to be used to generate the test data for the Spectral Processing element of the SPOC, the laboratory requirements for acquiring these spectra, and the sample analysis plan for acquiring the ancillary data required to properly interpret each spectrum.

The SAWG was tasked with delivering a report describing the minerals and chemicals detected using spectral-parameter analysis on simulated OVIRS data and the relative abundances of phases determined using linear deconvolution analysis of simulated OTES data. The CMWG focus was to determine whether or not these tests were successful by comparing the species determined by spectral analysis to the petrographic characterization of the unknowns following completion of the spectral tests. The CMWG was charged with preparing a report on the outcome of the test and delivering it to the PI Office. This report will inform next-step decisions that may trigger additional Phase C/D activities.

An evaluation team was assembled to prepare the Spectral Test Report. The team members were Neil Bowles, Kerri Donaldson Hanna, Lucy Lim, Ed Cloutis, Tim McCoy, Devin Schrader, and Lindsay Keller (chair). In addition, Keiko Nakamura-Messenger and Harold Connolly were *ex officio* members of the team.

What worked, what did not work, and why.

VNIR Results

The Evaluation team was impressed with the VNIR results (Tables 1, 2). Overall the VNIR analyses correctly resolved the analog samples and meteorite samples into hydrous and anhydrous groups where hydrous or anhydrous minerals are major constituents. Another success was in the detection of minor organics: VNIR correctly identified organics in the analog samples at the 5% level with only 2 false positives (at the trace level). VNIR detection of other minor phases at the 5% level was mixed. The VNIR results correctly identified the 5% addition of calcite in 4 of 4 samples, but gave a false positive on 1 sample. VNIR analyses detected the 5% addition of phyllosilicates in 2 of 2 samples, but gave 1 false positive. Pyroxene was identified in 3 of 5 samples at the ~10 wt. % level but were falsely identified in two other samples, a result not much better than chance. VNIR did not detect the 5% olivine present in the single hydrated analog test sample that contained olivine and also identified a sample with 66% olivine as “trace”. Not surprisingly, transparent minerals and minerals lacking strong, distinctive absorption features in the visible/near-IR were not detected in the VNIR analyses, including: plagioclase, FeNi metal, troilite, and magnetite.

No organic bands were detected in any of the meteorite samples, despite the fact that several of the samples (e.g. Murchison, Orgueil) contain 3-5% carbon in bulk. The spectra were collected under ambient conditions and the broad absorbed water feature may have attenuated the organic bands. Sample heterogeneity may also have affected the results.

For the VNIR, the generally better performance of the spectral metrics on the analog mixtures versus the carbonaceous chondrites (CC) is not surprising. Mechanical mixtures of the phases present in CCs cannot reproduce the spectra of corresponding CCs. This arises from the fact that the opaques in CCs are intimately associated with the clays at the submicron scale, and that texture is not well reproduced

in mechanical mixtures; therefore, absorption bands in mechanical mixtures will persist to much higher levels of opacities than are present in CCs. Phyllosilicate/silicate absorption bands in CC spectra are much shallower than in the corresponding mechanical mixture spectra. As a result, given the 5% band depth detection cutoff, CC spectra will often “fail” the test of detection of components with absorption bands.

Another factor working against detection of some minerals in both CC and analog mixture spectra is the nature of the 1 μm region. In many CC spectra we see a broad region of absorption here, and it is difficult to separate out or identify absorption bands due to specific phases. The 1 μm region contains contributions from multiple phases, including common CC phases that have an absorption feature in this region such as: magnetite (broad shallow band centered near 1 μm), Fe-bearing clays (particularly serpentine), with bands near 0.95 and 1.1 μm ; and an additional, common ferric-ferrous band around 0.75 μm , olivine with a main band around 1.05 μm plus a shoulder around 1.25 μm , pyroxene whose main band occurs around 0.9 μm (the 2 μm band of pyroxenes is usually weaker and hence often less detectable in CC spectra), and Fe sulfides, many having a broad band around 0.9-1 μm . Simple metrics cannot fully separate the relative contributions, and Gaussian curve fitting may not work because that analysis requires high signal to noise spectra to see subtle structure in the 1 μm region.

Given that temperature effects on VNIR spectra of carbonaceous chondrites are typically more subtle compared to spectral differences due to sample heterogeneity we do not endorse the SAWG recommendation to measure VNIR spectra over a range of temperatures. Temperature does have an effect on mafic silicate absorption bands and can alter their band minima and widths as observed in lab spectra of pure end members. However, given that silicate absorption features are shallow and broad in CC reflectance spectra, it is not expected that temperature effects could be separated from all the other variables that affect the 1 μm region in CC spectra. We note that Hinrichs and Lucey (2002) obtained a temperature series run on two CCs (Warrenton and Murchison) and the spectral differences in terms of absorption band shapes and positions were subtle across the 80 to 400K interval.

The samples used in the blind test represent a best-case scenario in terms of their “freshness”, but regolith samples from Bennu will likely exhibit absorption features in the VNIR that have been modified or destroyed by space weathering processes. We recommend a literature survey on the role of space weathering and its effect on VNIR reflectance spectra, especially on key features, especially organics and carbonates, that are known to be susceptible to damage and alteration by irradiation and impact processes (e.g. Brunetto et al. 2014). The literature survey should identify key knowledge gaps and suggest targeted experiments to address those gaps, e.g. simulated solar wind alteration of meteoritic organic matter.

TIR Results

The Evaluation team also evaluated the TIR results (Tables 3, 4). Overall the TIR analyses correctly resolved the analog samples and meteorite samples into hydrous and anhydrous groups where hydrous or anhydrous minerals are major constituents. In the TIR analyses, major olivine and phyllosilicates were consistently identified, but pyroxene and plagioclase present in the analog samples at the 10 wt.% level went undetected. TIR detection of minor phases at the 5% level was unreliable. Magnetite was correctly identified (as “oxide”) in 4 of 5 hydrated analog samples, but false positives were reported in 4 of 5 anhydrous analog samples. TIR analyses correctly indicated calcite in 4 of 4 samples where it was present at the 5 wt.% level, but generated 4 false positives where calcite was absent. Phyllosilicates (at the 5% level) in the anhydrous analogs was correctly detected in 1 sample, not detected in 1 sample, and gave a false positive in another. Thus, the phyllosilicate, magnetite and calcite results were little

better than random chance. Apparently, no information was gleaned from the TIR data for organic features. We recommend that TIR data should be obtained from the analog organic matter that was prepared for the blind test and be added to the spectral library. We also recommend that some thought should go into coordinating the VNIR and TIR analyses so that each benefits from their respective insights. This approach might help to resolve some of the ambiguities, even if at the level of a set of mutual spectral indices.

The SAWG report indicates that the derived mineralogy results obtained using the TIR linear unmixing model are not of sufficient quality at this time to permit an assessment of phase detectability at the 5% level. This is due in large part to the fact that the official ASU spectral library does not include fine particulate end members (<~65-75 μm), whereas the spectral features of the Blind Test spectra are dominated by fine particulates. We note however, that using existing fine particulate spectra from the literature (Run#4 of the SAWG report) still results in poor overall fits and additional false positives for mineral phases not present in the samples. The SAWG report concludes that without proper end members that match the particle size, chemistry, and crystallinity of the phases present in the test samples, or that match the phases expected to be present on the surface of Bennu, then quantitative analysis is not appropriate. It is unknown at this time whether the improvements to the spectral libraries would improve the results of the spectral test. *We recommend that the level-2 requirements (detection of key mineral phases at the 5% level) be revisited in order to assess the impacts to other aspects of the mission if the level-2 requirements cannot be met. The CMWG considers this result a distinct possibility given the outcome of the blind test.*

We agree with the SAWG recommendation that spectra of finer particle fractions of minerals should be added to the spectral library. Building a database of currently existing emissivity spectra of fine particulate minerals measured under ambient and SAE conditions will guide the necessary spectral library building activities. Ambient (N₂ atmosphere, ~1 bar) spectra of the Blind Test mixtures and meteorites were provided to the SAWG along with the SAE spectra. Running the linear unmixing algorithm using finer particle mineral spectra on the ambient spectra of the Blind Test mixtures and meteorites would be beneficial for better understanding the limitations of (a) the mineral end members in Hamilton's finer particle size fraction library and (2) the linear unmixing algorithm in determining modal mineral abundances of fine particulate samples when there are differences between particle size fractions (Blind Test mixtures and meteorites versus library end members).

The complexity inherent in carbonaceous chondrite meteorite samples (and hopefully at Bennu) means that any additions to the spectral library will need to be very carefully assessed, beyond just some finer particle fractions for the bulk minerals and non-mineral phases. (a) The perceived need to make measurements under a simulated asteroid environment (SAE) is built on the initial meteorites measured in the Pilot Study as well as the meteorites measured for the Blind Test (6 of the 7 meteorite spectra have thermal gradient effects when measured under SAE conditions). (b) We agree that the library needs to be built up with additional phases and particle size fractions using the components in the carbonaceous chondrites used in the Pilot Study and Blind Tests as guides. One possibility is to measure a range of carbonaceous chondrite meteorites at varying particle size fractions with known compositions and then use these as the spectral library end members. (c) ***Until we bring the sample back to Earth, we will not know the exact particle size distribution on Bennu so it seems unrealistic to measure a large (e.g. >4) set of particle size separates for every mineral or phase of interest.*** It seems more reasonable to measure a few particle size fractions for a few minerals or phases of interest and constrain the associated errors in modelling the modal mineral abundances of one or two of the Blind Test samples with the incorrect particle size fractions. The same is true regarding the mineral chemistries of the minerals on Bennu, so it is likely to be unfeasible to add every mineral chemistry

possible to the library, but understanding how a relatively imperfect composition affects the estimated modal mineral abundances is feasible.

We recommend a targeted study on the effects of particle size and mineral chemistry on linear unmixing of fine particulate samples. Using the known constituents of the Blind Test mixtures or other selected analogs, prepare 4 to 5 particle size fractions (e.g. < 25 μm , 25-75 μm , 75-125 μm , 125-250 μm , and > 250 μm) of 2 or 3 of the mixture constituents (e.g. olivine, pyroxene, phyllosilicate) and measure them under ambient conditions. SAE measurements should be included for a subset based on the experience gained from the existing test dataset. End member spectra can then be used to determine if this improves the linear unmixing results, and eliminate particle size fractions that do not greatly improve the results (e.g. what is the trade off in modal mineralogy for simplifying the number of particle size fractions added to the spectral library? Essentially, only include size fractions with a demonstrated effect on spectral shape). A similar approach could be used to explore the spectral variability that arises from mineral chemistry for selected phases. These analyses and results will inform future sample preparation for continued work on a defined spectral library. It will also further constrain how well the linear unmixing algorithm can work for determining modal mineralogies for samples with unknown particle size distributions.

It is clear from the SAWG analyses of the Blind Test mixtures and meteorites that the spectral library needs additional phases to fully represent minerals/materials found in a range of carbonaceous chondrite meteorites, in particular the CM chondrites that may be representative of Bennu. The SAWG has recommended μ -FTIR reflectance measurements of sub-components of meteorite analogs to improve the library coverage. However, there are several issues with this approach. Even with the stated spatial resolution of the μ -FTIR reflectance measurements, multiple phases will be contributing to the spectrum given the typical fine-grained nature of hydrated CC matrix, so single phase spectra of fine-grained alteration phases will be difficult or impossible to obtain. It is unclear how the μ -FTIR reflectance measurements will improve the linear unmixing algorithm results if they do not exhibit the correct particle size? It is also unclear that the measured per-grain reflectance can be related/scaled to an appropriate (regolith) emissivity spectrum. The μ -FTIR reflectance measurements would be useful in conjunction with other coordinated analyses in understanding the modal mineralogy of the meteorite samples.

Similar to the VNIR discussion above, space weathering effects on TIR spectra should be investigated through a literature survey and possible experiments. Solar wind exposure is known to cause amorphization and band shifts in some irradiated silicate materials (Lantz et al. 2015), but this is an area of active research. Amorphous materials in general were not part of the spectral test, but potentially will be an important component to consider for a primitive body like Bennu. This highlights the importance of the CMWG project on preparation and characterization of analogs and meteorites with a significant amorphous silicate component e.g. what is the range in particle size for serpentine where it is not possible to spectrally differentiate it from truly amorphous serpentine formed by irradiation or thermal metamorphism?

Modal Mineralogy of Meteorite Samples: PSD-XRD.

One complication for the spectra test was the lack of quantitative modal mineralogy for the meteorite samples. The CMWG plan was to use position-sensitive detector x-ray diffraction (PSD-XRD) to obtain the quantitative mineralogy of the samples. To this end, three sub-samples of the analog samples were analyzed as a “blind test” of the PSD-XRD results. The results of this blind test were summarized in the report “Spectral Analysis Science Analog Report: PSD-XRD Results” submitted to the CMWG. The major

conclusion from that test was that the PSD-XRD analyses failed to reproduce the mineralogy and abundances of phase in the mixtures. We have subsequently reviewed the analyses in consultation with Sara Russell and Ashley King, and now understand how erroneous interpretations of the patterns affected the results. Russell and King have re-analyzed the original data and now are achieving excellent agreement with the measured mineralogy. The seven meteorite samples are being sent to Russell and King and we anticipate delivery of the quantitative data by late January 2016. As soon as these data are available, they will be forwarded to the SAWG. We also recommend that additional independent measurements of modal mineralogy of the meteorite samples be obtained through additional analytical means (e.g. point-counting of thin sections in the electron microscope/microprobe, μ -FTIR reflectance measurements, etc.) to validate the PSD-XRD results.

References:

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Table 1. A comparison of the VNIR results with the actual components in the anhydrous and hydrated analog samples. (Y=positive detection, Y=false positive, n.d.=not detected, ?=value close to threshold, visually verified, trace=below threshold but visually verified).

| Anhydrous Analogs Names | Bruce | | Tony | | Natasha | | Bucky | | Selina | |
|----------------------------|--------|--------|--------|-------|---------|------|--------|--------|--------|------|
| | wt% | VNIR | wt% | VNIR | wt% | VNIR | wt% | VNIR | wt% | VNIR |
| Olivine | 70.00 | Y | 66.50 | trace | 66.50 | Y | 66.50 | Y | 59.50 | Y |
| fine (85%) | | | | | | | | | | |
| coarse (15%) | | | | | | | | | | |
| Pyroxene (85% LCP, 15%HCP) | 10.00 | Y | 9.50 | Y | 9.50 | n.d | 9.50 | Y | 8.50 | n.d |
| LCP | | | | | | | | | | |
| fine (85%) | | | | | | | | | | |
| coarse (15%) | | | | | | | | | | |
| HCP | | | | | | | | | | |
| Plagioclase | 10.00 | n.d | 9.50 | n.d | 9.50 | n.d | 9.50 | n.d | 8.50 | n.d |
| Fe,Ni-metal | 5.00 | n.d | 4.75 | n.d | 4.75 | n.d | 4.75 | n.d | 4.25 | n.d |
| troilite | 5.00 | n.d | 4.75 | n.d | 4.75 | n.d | 4.75 | n.d | 4.25 | n.d |
| Organics | | trace? | | n? | 5.00 | Y | | trace? | 5.00 | Y |
| magnetite | | | | | | | | | | |
| Ca-carbonate (calcite) | | | 5.00 | Y | | n? | | | 5.00 | Y |
| Phyllosilicate (50%, 50%) | | | | | | Y | 5.00 | y | 5.00 | Y |
| Saponite | | | | | | | | | | |
| Lizardite | | | | | | | | | | |
| Total | 100.00 | | 100.00 | | 100.00 | | 100.00 | | 100.00 | |
| | | | | | | | | | | |
| Hydrated Analogs Names | Steve | | Clint | | Peggy | | Wanda | | Nick | |
| | wt% | VNIR | wt% | VNIR | wt% | VNIR | wt% | VNIR | wt% | VNIR |
| Olivine | | | | | | | 5.00 | n.d. | | |
| fine (50%) | | | | | | | | | | |
| coarse (50%) | | | | | | | | | | |
| Pyroxene (85% LCP, 15%HCP) | | | | | | Y | | | | Y |
| Plagioclase | | | | | | | | | | |
| Fe,Ni-metal | | | | | | | | | | |
| troilite | 5.00 | n.d. | 4.75 | n.d. | 4.75 | n.d. | 4.75 | n.d. | 4.25 | n.d. |
| Organics | | | | | 5.00 | Y? | | | 5.00 | Y? |
| magnetite | 5.00 | n.d. | 4.75 | n.d. | 4.75 | n.d. | 4.75 | n.d. | 4.25 | n.d. |
| Ca-carbonate (calcite) | | Y | 5.00 | Y | | Y | | | 5.00 | Y |
| Phyllosilicate (50%, 50%) | 90.00 | Y | 85.50 | Y | 85.50 | Y | 85.50 | Y | 81.50 | Y |
| Saponite (50%) | | | | | | | | | | |
| Lizardite (50%) | | | | | | | | | | |
| Total | 100.00 | | 100.00 | | 100.00 | | 100.00 | | 100.00 | |

Table 2. VNIR results on blind test meteorite samples.

| Sample names | Meteorite | VNIR results |
|---------------------|---------------------------|---|
| Shepard | Allende (CV3oxA) | anhydrous, trace olivine |
| Grissom | Farmington (L5 – shocked) | anhydrous, pyroxene |
| Glenn | Murchison (CM2) | hydrated, phyllosilicates |
| Carpenter | MIL 090001 (CR2) | hydrated, phyllosilicates, olivine, calcite |
| Schirra | ALH 83100 (CM1/2) | hydrated, phyllosilicates, olivine |
| Cooper | Orgueil (CI) | hydrated, phyllosilicates, calcite |
| Slayton | Vigarano (CV3red) | anhydrous, trace pyroxene |

Table 3. A comparison of the TIR results with the actual components in the anhydrous and hydrated analog samples. (Y=positive detection, Y=false positive, ? = additional uncertainty, n.d.=not detected).

| Anhydrous Analogs Names | Bruce | | Tony | | Natasha | | Bucky | | Selina | |
|----------------------------|--------|------|--------|------|---------|------|--------|------|--------|------|
| | wt% | TIR | wt% | TIR | wt% | TIR | wt% | TIR | wt% | TIR |
| Olivine | 70.00 | Y | 66.50 | Y | 66.50 | Y | 66.50 | Y | 59.50 | Y |
| fine (85%) | | | | | | | | | | |
| coarse (15%) | | | | | | | | | | |
| Pyroxene (85% LCP, 15%HCP) | 10.00 | n.d | 9.50 | n.d | 9.50 | n.d | 9.50 | n.d | 8.50 | n.d |
| LCP | | | | | | | | | | |
| fine (85%) | | | | | | | | | | |
| coarse (15%) | | | | | | | | | | |
| HCP | | | | | | | | | | |
| Plagioclase | 10.00 | n.d | 9.50 | n.d | 9.50 | n.d | 9.50 | n.d | 8.50 | n.d |
| Fe,Ni-metal | 5.00 | n.d | 4.75 | n.d | 4.75 | n.d | 4.75 | n.d | 4.25 | n.d |
| troilite | 5.00 | n.d | 4.75 | n.d | 4.75 | n.d | 4.75 | n.d | 4.25 | n.d |
| Organics | | | | | 5.00 | | | | 5.00 | |
| magnetite | | Y | | | | Y | | Y | | Y |
| Ca-carbonate (calcite) | | Y | 5.00 | Y | | | | Y | 5.00 | Y |
| Phyllosilicate (50%, 50%) | | | | | | Y | 5.00 | n.d. | 5.00 | Y |
| Saponite | | | | | | | | | | |
| Lizardite | | | | | | | | | | |
| Total | 100.00 | | 100.00 | | 100.00 | | 100.00 | | 100.00 | |
| | | | | | | | | | | |
| | | | | | | | | | | |
| Hydrated Analogs Names | Steve | | Clint | | Peggy | | Wanda | | Nick | |
| | wt% | TIR | wt% | TIR | wt% | TIR | wt% | TIR | wt% | TIR |
| Olivine | | Y? | | Y? | | Y? | 5.00 | Y? | | Y? |
| fine (50%) | | | | | | | | | | |
| coarse (50%) | | | | | | | | | | |
| Pyroxene (85% LCP, 15%HCP) | | | | | | | | | | |
| Plagioclase | | Y? | | Y? | | Y? | | Y? | | Y? |
| Fe,Ni-metal | | | | | | | | | | |
| troilite | 5.00 | n.d. | 4.75 | n.d. | 4.75 | n.d. | 4.75 | n.d. | 4.25 | n.d. |
| Organics | | | | | 5.00 | | | | 5.00 | |
| magnetite | 5.00 | Y | 4.75 | Y | 4.75 | Y | 4.75 | n.d. | 4.25 | Y |
| Ca-carbonate (calcite) | | | 5.00 | Y | | Y | | Y | 5.00 | Y |
| Phyllosilicate (50%, 50%) | 90.00 | Y | 85.50 | Y | 85.50 | Y | 85.50 | Y | 81.50 | Y |
| Saponite (50%) | | | | | | | | | | |
| Lizardite (50%) | | | | | | | | | | |
| Total | 100.00 | | 100.00 | | 100.00 | | 100.00 | | 100.00 | |

Table 4. Modal Mineralogy of Meteorite Samples in Blind Test Compared with TIR Results. The modal mineralogy presented here were taken from literature data because quantitative results from the actual blind test samples have not yet been obtained.

| | Slayton | Slayton | Shepard | Shepard | Glenn | Glenn | Schirra | Schirra | Cooper | Cooper | Grissom | Grissom | Carpenter | Carpenter |
|---------------|----------|----------|---------|---------|-----------|-----------|----------|----------|---------|---------|-----------|-----------|-----------|-----------|
| | Vigarano | Vigarano | Allende | Allende | Murchison | Murchison | ALH83100 | ALH83101 | Orgueil | Orgueil | Farmingto | Farmingto | MIL090001 | MIL090001 |
| | Vol% | TIR | Vol% | TIR | Vol% | TIR | Vol% | TIR | Vol% | TIR | Wt% | TIR | | TIR |
| Olivine total | 85 | X | 82.7 | X | 15.1 | X | 8.7 | err | 1 | X | 42.2 | X | Y | X |
| Enstatite | 8.1 | X | 6.3 | | 8.3 | | 0.7 | | | X | 31.9 | X | Y | X |
| Anorthite | 1.1 | | 1.1 | | | | | | | | 9.3 | | | |
| Magnetite | 1.4 | X | 0.3 | | 1.1 | | 1.7 | X | 6.7 | X | | err | y | err |
| Fe Sulfide | 2.4 | | 6.6 | | 1.9 | | 1 | | 5.7 | | 6.8 | | y | |
| FeNi metal | 2 | | 1 | | | | | | | | 9 | | y | |
| Phyllos | 0 | X | 1.9 | X? | 72.5 | X | 86.6 | X | 83 | X | | X? | Y | X |
| Calcite | | X | | X | 1.2 | X | 1.2 | X | | X | | X | y | X? |
| Ferrihydrite | | | | | | | | | 3.3 | | | | | |
| Total | 100 | | 99.9 | | 100.1 | | 99.9 | | 96.4 | | 99.2 | | | |

1: PSD-XRD modal mineralogy For CV, CM and CI chondrites from Howard et al. 2010, 2011, 2015.

2: Data for Farmington are estimated using the "average L5" value from Dunn et al. 2010.

3: Data for Farmington are in wt%, the rest are in vol%.

4: Data for MIL 090001 from Keller et al 2011 - Present/Absent, Y=major, y=minor

5: Black Xs indicate a detection (>5%) by linear mixture modeling that is confirmed by visual inspection.

6: Orange Xs indicate detections (>5%) by linear mixture modeling that may be unreliable due to poor fit quality and cannot be confirmed with certainty by visual inspection.

7: Red Xs are detections by visual inspection only. Question marks indicate an additional level of uncertainty.

8: Cells with "err" indicate a detection by the linear least squares model (>5%) where the uncertainties exceed the modeled abundance.

Spectral Test Plan Sample Mixtures November 2015

| Anhydrous Analogs | Bruce | Tony | Natasha | Bucky | Selina |
|----------------------------|---------------|---------------|----------------|---------------|---------------|
| | wt% | wt% | wt% | wt% | wt% |
| Olivine | 70.00 | 66.50 | 66.50 | 66.50 | 59.50 |
| fine (85%) | | | | | |
| coarse (15%) | | | | | |
| Pyroxene (85% LCP, 15%HCP) | 10.00 | 9.50 | 9.50 | 9.50 | 8.50 |
| LCP | | | | | |
| fine (85%) | | | | | |
| coarse (15%) | | | | | |
| HCP | | | | | |
| Plagioclase | 10.00 | 9.50 | 9.50 | 9.50 | 8.50 |
| Fe,Ni-metal | 5.00 | 4.75 | 4.75 | 4.75 | 4.25 |
| troilite | 5.00 | 4.75 | 4.75 | 4.75 | 4.25 |
| Organics | | | 5.00 | | 5.00 |
| magnetite | | | | | |
| Ca-carbonate (calcite) | | 5.00 | | | 5.00 |
| Phyllosilicate (50%, 50%) | | | | 5.00 | 5.00 |
| Saponite | | | | | |
| Lizardite | | | | | |
| Total | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 |

| Hydrated Analogs | Steve | Clint | Peggy | Wanda | Nick |
|----------------------------|---------------|---------------|---------------|---------------|---------------|
| | wt% | wt% | wt% | wt% | wt% |
| Olivine | | | | 5.00 | |
| fine (50%) | | | | | |
| coarse (50%) | | | | | |
| Pyroxene (85% LCP, 15%HCP) | | | | | |
| Plagioclase | | | | | |
| Fe,Ni-metal | | | | | |
| troilite | 5.00 | 4.75 | 4.75 | 4.75 | 4.25 |
| Organics | | | 5.00 | | 5.00 |
| magnetite | 5.00 | 4.75 | 4.75 | 4.75 | 4.25 |
| Ca-carbonate (calcite) | | 5.00 | | | 5.00 |
| Phyllosilicate (50%, 50%) | 90.00 | 85.50 | 85.50 | 85.50 | 81.50 |
| Saponite (50%) | | | | | |
| Lizardite (50%) | | | | | |
| Total | 100.00 | 100.00 | 100.00 | 100.00 | 100.00 |

Meteorite Samples

| | |
|----------------|-----------------------------------|
| Shepard | Allende (CV3oxA) |
| Grissom | Farmington (L5 – shock blackened) |
| Glenn | Murchison (CM2) |

Carpenter

MIL 090001 (CR2)

Schirra

ALH 83100 (CM1/2)

Cooper

Orgueil (CI)

Slayton

Vigarano (CV3red)

Spectral Science Test Data

The SAWG prepared a report on their analysis of the test spectra, and an evaluation team from the CMWG assessed the SAWG results.