Constraining the Origin of the Jupiter Trojans by In Situ Measurement of Volatiles, Minerals, and Ices

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Bold = Primary participants, meeting bi-weekly * = Heavy Participation

2 EXECUTIVE SUMMARY

As the KISS Trojans program comes to a close, we report here on our achievements in this venture that began with a KISS workshop in 2012, "*In Situ Science and Instrumentation for Primitive Bodies*". The original workshop brought together a diverse group (see Appendix B) that set out to tackle an ambitious goal – to find a way to test predictions of dynamical models (such as the Nice model, named after the founding research group in Nice, France), that have recently led to a radically new understanding of solar system formation. We aimed to do so through interdisciplinary collaboration between the planetary dynamics communities that have formulated (and largely dominated discussion of) these new ideas, and the meteoritics and cosmochemistry communities who would no doubt be involved in any *in situ* mission to an outer solar system body.

At the start of our study, we found that while both of these communities had well-formed and consequential hypotheses about solar system evolution, they had been developed essentially independently. It was not obvious that either community was equipped to make a concrete statement testable by the other. Our study therefore became principally focused on bringing these communities together to come up with explicit tests of the predictions of these new dynamical models of solar system evolution. In retrospect, it has become apparent that this study was indeed timely. As we pursued the ideas developed in the first and second workshops, it became clear to the group as a whole that focusing specifically on the Trojan asteroids of Jupiter, a large and ancient population of small bodies trapped in the Sun-Jupiter gravitational L4 and L5 Lagrange points, presented an opportunity to focus on a key reservoir of primitive bodies that are thought to be linked to the early dynamical evolution of the outer solar system, potentially sharing the same parent source as Kuiper Belt Objects. Through lively debate that largely marked both workshops, the idea of the Trojan asteroids as a test case for origins, though not new (e.g. see Trojan Tour Decadal Study, Brown 2010), was becoming socialized among key planetary scientists who then rallied around this concept, despite much initial skepticism. Indeed, the existence of this KISS program, and its timely nature, has played a vital role in bringing Trojan asteroid origins into the forefront of planetary science. As a consequence, this KISS study (though certainly not solely responsible) was highly influential in the proposal and subsequent selection of NASA's Lucy Discovery mission concept to the Jupiter Trojans (Levison *et al.,* 2017). Several key participants in Lucy, including Hal Levison (Lucy Principal Investigator *AND* Distinguished Visiting Scientist of the initial KISS Study), were a vital part of those initial debates which ultimately led to the consensus that the Trojans are a key to unlocking origins.

Our current KISS program that has now come to a close, "*Constraining the Origin of the Jupiter Trojans by In Situ Measurement of Volatiles, Minerals, and Ices*", uses theory and experiment to come up with a set of chemical markers of solar system origins. We set out to do this work with the idea that the search for these markers would then be the basis of the science motivation for future missions to these bodies. With the Lucy mission concept, the first reconnaissance of the

Jupiter Trojan asteroids, now expected to launch in 2021, we are presented with the possibility of realizing this goal far sooner than originally anticipated. Lucy would visit six Trojan asteroids covering the full range of observed taxonomic types. In this report, we describe in detail our predictions about the chemistry of the surface of the Trojans, and supporting results of laboratory and telescopic studies. The hypotheses presented here could be directly tested through the investigations performed during Lucy's many encounters with the Trojans.

3 INTRODUCTION

3.1 ORIGINS

The Trojan asteroids inhabit the L4 and L5 Lagrangian regions of the Jupiter-Sun system. The source of the current Trojan population is unknown, though they are thought to be survivors of the population of planetesimals that existed in the primordial disk when the giant planets formed. This current understanding is derived from predictions made by recent dynamical models (Morbidelli *et al.* 2005; Nesvorný *et al.* 2013). In this framework, both the Jupiter Trojans and the Kuiper belt objects are derived from the same source populations – these early planetesimals that existed prior to the dynamical instability – and their separate locations today are a result of their different dynamical histories.

While the dynamical connections between early planetesimals, Jupiter Trojans, and Kuiper belt objects have become well accepted, connecting these two populations based on observables has been challenging. Little is known compositionally about the Jupiter Trojans which have been characterized by featureless red spectra, typically explained by the expectation that their surfaces are highly weathered. Kuiper Belt objects on the other hand, due to their location in the outer solar system, retain ices such as water and methanol that have been observed on small objects (Barucci *et al.* 2011; Brown *et al.* 2012).

3.2 COMPOSITION & THE TWO TROJAN POPULATIONS

Efforts to gain compositional information on the Jupiter Trojans have focused on ground- and space-based telescopic observations in the visible through mid-infrared spectral regions. Observations in the visible to near infrared spectral region have revealed an intriguing clue to the composition of the Trojan asteroids, while also providing potential evidence for the connection between Trojans and objects in the Kuiper belt. The Trojans, like objects in the Kuiper belt, were found to be are comprised of two populations with distinct spectra (Emery *et al.,* 2011) as shown in Figure 1. Though both types of Trojan spectra are featureless, they can be classified into two groups designated "red" and "less-red" that differ in color but are completely mixed dynamically.

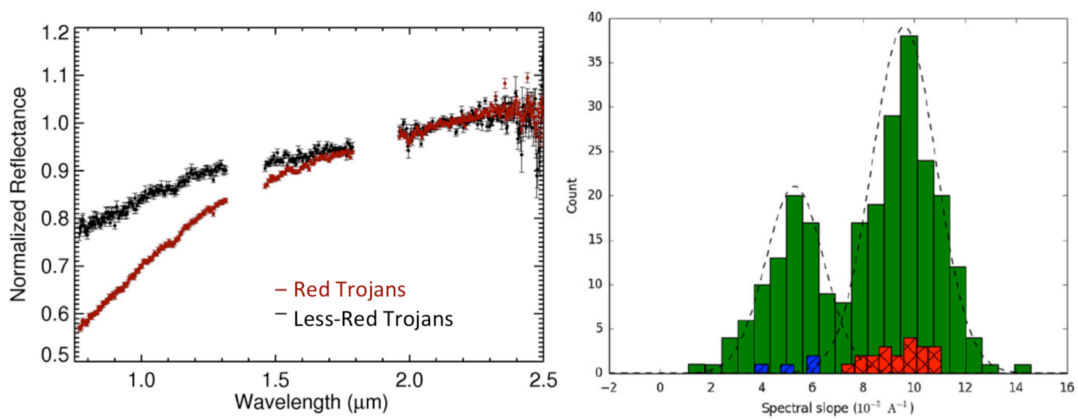

Figure 1. (left) Averages of visible to near infrared spectra of the two Trojan compositional groups (after Emery *et al.*, 2011). **(right)** Synthesis of data showing bimodal spectral slope distribution in the Trojan asteroids. The green bars represent 254 Trojans in the Sloan sample with H<12.3 and the red and blue represent 24 previously published Trojan spectral slopes (after Wong *et al*, 2014).

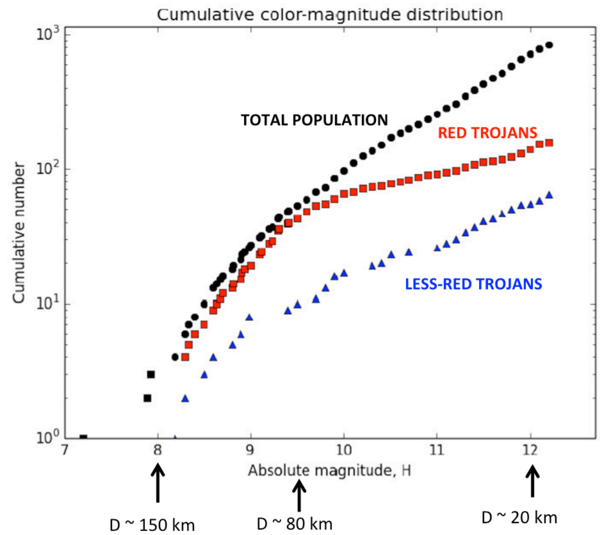

Figure 2. Plot of the cumulative magnitude distribution for the main Trojan sample from Wong *et al*., 2014. For reference, below the axis are several markers indicating the approximate Trojan asteroid diameter corresponding to the magnitude scale.

Furthermore, the two color populations were found to have magnitude distributions that are remarkably distinct (see Figure 2); this is an important clue suggesting that while the red and less-red Trojans comprise a single population, their formation likely occurred at distinctly different heliocentric distances within the primordial disk before being emplaced to their current location.

3.3 THE SULFUR HYPOTHESIS

While the reason for the two distinct color groups remains unknown, we have developed a hypothesis through this KISS program (detailed in Wong and Brown, 2016) that offers an explanation based on a difference in organic surface composition resulting from differing dynamical histories. At the heart of our hypothesis, as illustrated in Figure 3, is the idea that the bimodal distribution of colors began in the primordial planetesimal disk (between ~15 and 30 AU), and stems from location-dependent volatile loss in this region prior to the onset of the early giant planet dynamical instability. The presence of a sharp dividing line between red and less-red objects can be attributed to differences in heliocentric distance prior to the dynamical instability. As illustrated in Figure 3, on either side of the dividing line, objects either retained or lost H_2S on their surfaces over relevant timescales (~100 Myr). Subsequent irradiation then led to two distinctly different surfaces covered in non-volatile organic residue from the irradiation of ices–one with and one without sulfur—that are ultimately responsible for the two colors observed in the Kuiper belt today. At the time of emplacement after the dynamic instability, the primordial red and very-red objects became the KBOs, while the Trojan population experienced some color evolution, maintaining the bimodality but resulting in less-red colors. This hypothesis also offers an explanation for the observed depletion of the red- relative to the less-red Trojans for small sizes (Trojans with diameter less than ~80 km as evident in Figure 2) (Wong *et al*., 2014). In this scenario, since the red and less-red Trojans have identical interior composition, differing only in the their outer surfaces, shattering collisions in the red population would result in less-red surfaces as H_2S can not be retained under the current conditions. Therefore collisional fragments from both red and less-red objects would ultimately end up less-red.

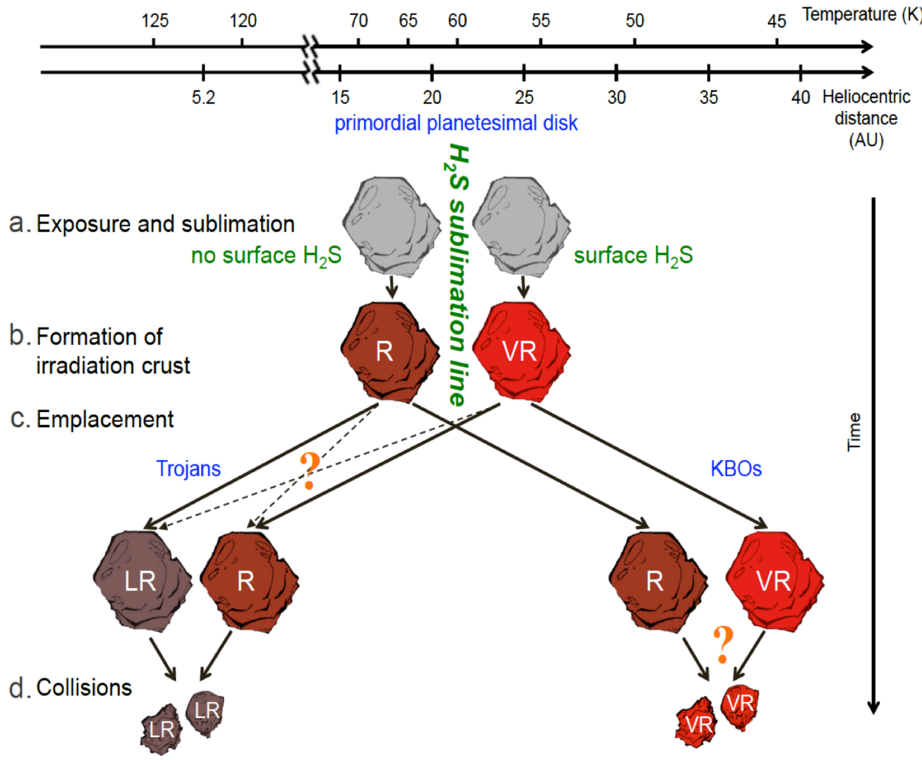

Figure 3. Representation of our hypothesized scenario where the presence and absence of H_2S is responsible for the very-red and less-red KBOs. The two KBO populations are formed in the primordial disk inside and outside of the H_2S evaporation line with exposure and sublimation dictated by heliocentric distance, leading to the formation of red and very-red nonvolatile irradiation crusts. When the large-scale solar system disruption occurs, these two populations are scattered in to their current locations, with one outcome being the two Trojan populations which become red and less-red through processing during and after emplacement. At the same time, the current KBO source populations remain and retain their original colors. Collisional fragments of the Trojans become less-red because freshly exposed H_2S on the surface is no longer stable.

The theory that H_2S is the most likely constituent responsible for the bimodal color distribution was postulated only after exploring other potential candidates, including all volatile ice species with average measured abundances relative to water greater than 0.5% as reported from comet comae measurements. In order of stability from longest to shortest retention time, these are: H_2O, CH_3OH, HCN, NH_3, CO_2, H_2S, C_2H_2, C_2H_6. While the exact assumptions made about irradiation time scales and surface layers may not be precise, and changes in these parameters alter the location of the individual sublimation lines, the order of stability of the volatiles remains accurate. For a wide range of assumptions, we found that H_2S is the most likely candidate responsible for the differences between the red and less-red objects. This also makes intuitive sense because sulfur is a known reddening agent, and the expected radial distance where H_2S becomes unstable is in a reasonable location in the primordial disk for the formation of the two KBO populations on both sides of the line. The only other candidate to consider would be ethane, however it is not considered a viable candidate because it is not expected to cause appreciable changes in reddening.

While features indicative of organics have not been previously observed on the Trojans, this could be due to the difficulty in making these measurements remotely on such faint dark objects. And in fact, as we will discuss later, our most recent Trojan asteroids observations have revealed weak spectral features near 3 μm that we postulate can be attributed to organics (Brown, 2016). It is the exploration of these organic residues that we propose are representative of Trojan asteroid surfaces that is the goal of our experimental work.

3.4 THE SILICATE HYPOTHESIS

An alternate hypothesis for the two distinct spectral groups focuses on differences in silicate composition rather than organics. In fact, the only spectral features on the Trojans that have been identified to date are the signatures of amorphous or fine-grained silicates as shown in Figure 4 (Emery *et al.* 2006). According to the most widely accepted disk models (e.g. Henning *et al.* 2010), a radial distribution in silicon in various silicate dust components is predicted (see Figure 5). There are three observable trends predicted with increasing heliocentric distance: (1) the crystalline/amorphous fraction decreases (2) the olivine/pyroxene ratio increases (3) the Fe/Mg ratio increases. Higher olivine content has been potentially linked to red slope (Vernazza et al., 2015) which is in agreement with the notion that the red Trojans formed in the outer part of the disk with higher olivine content than the less red Trojans which formed in the inner part of the disk. While this is a sensible line of reasoning, it is more difficult to come up with a plausible explanation for why the silicate composition is bimodal rather than gradually varying. One possibility is that gaps in the primordial disk were swept out of the disk by larger bodies prior to the time of planetesimal formation, leaving a gap in silicate content. More work must be done in order to determine whether this hypothesis holds up to closer scrutiny.

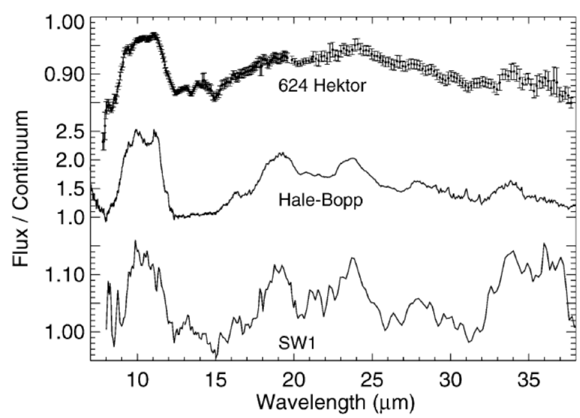

Figure 4. Emissivity spectrum of Hektor, a large member of the red Trojan spectral group shows features indicative of fine-grained or amorphous silicates. Similarities are evident between emissivity spectra of Trojans and comets Hale-Bopp and SW1.

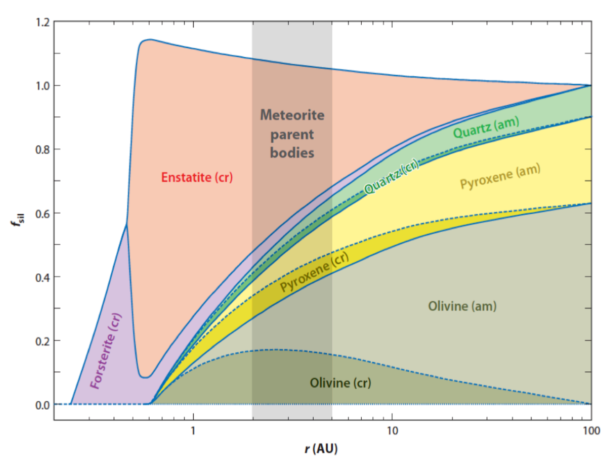

Figure 5. Radial distribution of silicon condensed in various silicate dust components (from Henning et al., 2010).

3.5 FUTURE OBSERVATIONS TO ELUCIDATE COMPOSITION AND CHEMISTRY

While the Trojans today are still shrouded in mystery, the future looks bright for gaining real insight into their composition and chemistry with the proposed Lucy mission that would perform spatially resolved measurements during 6 flybys and the James Webb Space Telescope which will be able to obtain whole body spectra with far greater sensitivity than we have today (Norwood *et al.,* 2016; Rivkin *et al.,* 2016). Our future goal is to compare results of our laboratory experiments with the compositional data that would be obtained by Lucy and JWST in order to test the hypothesis laid out in this work.

4 LABORATORY EXPERIMENTS

We devised a set of laboratory experiments designed to test the sulfur hypothesis described previously. The goal of these experiments was to produce simulants in the laboratory of ices relevant to the parent bodies that would have formed in the primordial disk, making a distinction between the inner and outer parts of the disk. These simulants were produced and then subjected to conditions --- irradiation and heating – to mimic as closely as possible the conditions experienced by these bodies during formation and migration.

These experiments were carried out in the Icy World Simulation Laboratory at the Jet Propulsion Laboratory. A detailed description of the facilities and capabilities of this laboratory can be found in Hand & Carlson (2011). The experimental setup was based on a high vacuum chamber with a base pressure of ~ 1 x 10^{-8} torr, as illustrated in Figure 6. The ices were grown on gold-coated glass substrates attached to a cold finger on a closed-cycle helium cryostat. An external manifold was used to prepare gas mixtures prior to deposition. The ice films were grown by leaking the gas mixture into the chamber, forming ices on a gold mirror that was held at 50 K. Most of the gas deposited directly, but a small fraction did not, resulting in a rise of chamber pressure of a few 10^{-8} torr. For irradiation experiments, an electron gun (monitored by a faraday cup) produced high-energy electrons (10 keV) directed at the ice with a typical beam current of 0.5 μ A.

We began by simulating mixtures of ices relevant to the parent bodies that would have formed in the primordial disk. Using combinations of these four ices -- H_2O, CH_3OH, NH_3, and H_2S -- we produced simulants, processed them by irradiation, and characterized them for chemical and spectral properties. A typical experimental process is shown in Figure 7, and the ice compositions and irradiation conditions are shown in Figure 8.

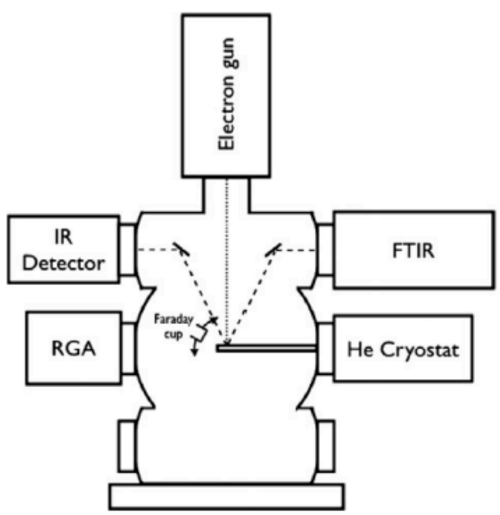

Figure 6. Diagram showing the chamber configuration.

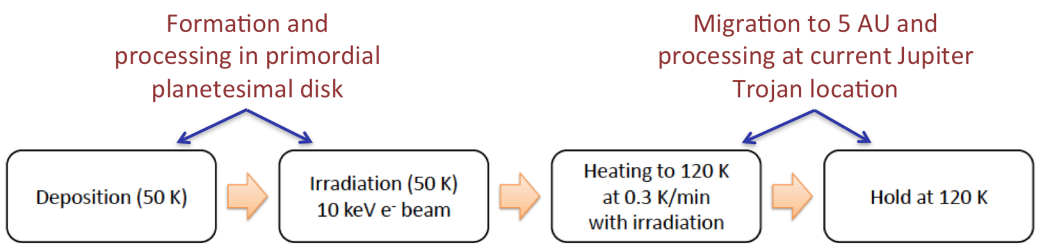

Figure 7. Typical experimental process for ice simulants.

Composition of ice mixtures as deposited:
4 ice Mixture: $MeOH-NH_3-H_2S-H_2O$ = 3:3:3:1
3 ice Mixture: $MeOH-NH_3-H_2O$ = 4:4:2
*** keeping the same $MeOH/NH_3$ ratio in both mixtures.**

IRRADIATION CONDITIONS FOR ICE MIXTURES		
Electron Fluence	**Corresponding solar e^- irradiation time at 5 AU**	**Corresponding solar e^- irradiation time at 15 AU**
~ 2×10^{21} eV/cm^2	~ 200,000 Yrs	~ 1.8 Million Yrs

Figure 8. Composition of ice mixtures and irradiation conditions used in our experiments. The 3-ice mixture does not contain sulfur and the 4-ice mixture contains sulfur in the form of H_2S ice.

5 OUTCOME OF THE PROGRAM

5.1 LABORATORY RESULTS

We have performed a series of experiments designed to test the hypothesis that sulfur is the relevant reddening agent. A summary of the relevant findings follows:

Spectral properties of irradiated ices

Because sulfur is a known reddening agent, we expected to observe a marked reddening in the 4-ice (with-H_2S) mixture as compared to the 3-ice (without H_2S) mixture. This is indeed what was observed as shown in Figure 9. While this is an important observation, it is only the first piece of the puzzle.

The next step was to look at the chemical and spectral properties of the organic residues formed in these ices after irradiation and heating, and evaluate whether chemical differences could account for the spectral differences observed in the Trojan asteroids. Along with the marked reddening that occurs, chemical changes are clearly evident between the 3-ice and 4-ice mixtures (see Figure 10 and Figure 11). More detail is available in Mahjoub *et al.* (2016). To summarize, when H_2S is included in the starting mixture, OCS is one of the sulfur-containing products formed after irradiation. Upon heating we also see an increase in CS and SO_2. The sulfur products remain after heating to Trojan temperatures – a sign that these products represent a non-volatile component that would remain on the surface after ices are processed.

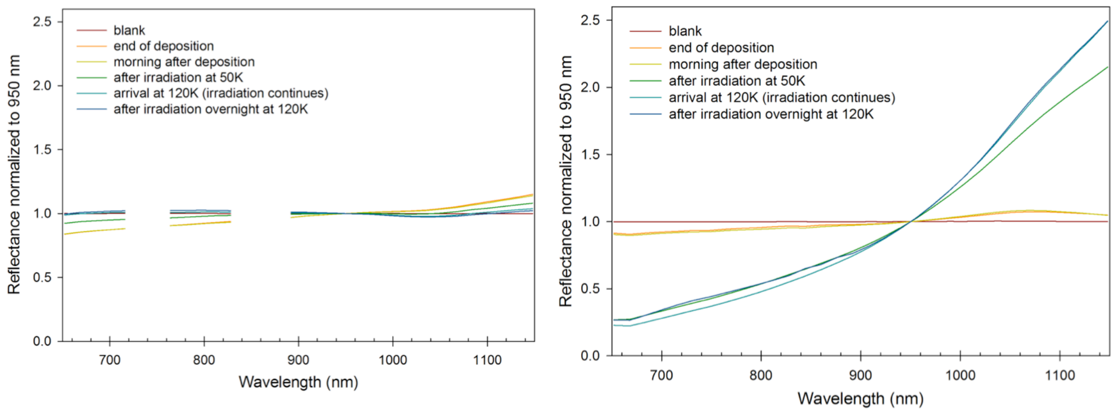

Figure 9. Reflectance measurements of 3 ice (top) and 4 ice (bottom) mixtures at various stages in the irradiation experiment. The key feature to note is the marked reddening which occurs in the 4 ice mixture (containing H_2S) after irradiation at 50K. When warming to 120K (simulating the current Trojan location) that reddening does not disappear, indicating that non-volatile products have formed that could be responsible for the reddening of the Trojan asteroids as observed today.

Spectral properties of non-volatile residues

Finally, we collected spectra of the products remaining after heating ices to room temperature. While not representative of real Trojan temperatures, this allowed us to analyze the non-volatile residues using characterization techniques not available to us in the ice deposition chamber. Since we know that thermal processing can occur between 120K and 300K, we must keep in mind that the products we have analyzed may contain some differences from residues remaining at lower temperature. Still, we can learn from these results.

When characterized at room temperature, the overall appearance of the infrared spectrum changed drastically with the addition of sulfur (see Figure 12). Notably, overall contrast in the spectrum was greatly reduced with the addition of sulfur. Three main differences were observed between the 3-ice and 4-ice mixtures. When sulfur was present, the production of sulfur-rich polymers is indicated, and there is a decrease in both the CN band and the NH_x band. This supports the conclusion that sulfur dramatically impacts the overall chemistry of the non-volatile residues, inhibiting the formation of many organic compounds.

Temperature programmed desorption (TPD)

Temperature Programmed Desorption (TPD) of the irradiated mixtures allowed us to detect small sulfur allotropes (S_2, S_3 and S_4) that formed after irradiation of our H_2S containing ice mixtures, and are known to be red in color These small red polymers are metastable and could polymerize further under thermal processing and irradiation, producing larger sulfur polymers (mainly S_8) that are spectroscopically neutral at wavelengths above 500 nm (Meyer *et al.,* 1971, 1976; Baklouti *et al.,* 2008). This transformation of sulfur species could be the basis for objects from the primordial planetesimal disk becoming less red after emplacement and exposure to elevated temperature (i.e why Trojans are less red than KBOs). Along with allotropes, we observed production of organo-sulfur molecules ($(CH_3)_2S$, $(CH_3)_2S_2$). The production of these compounds reveals a rich carbon sulfur chemistry that, as a side note, may have an important prebiotic interest. Results of our TPD experiments are described in detail in Mahjoub *et al.*, 2017(*submitted to ApJ*).

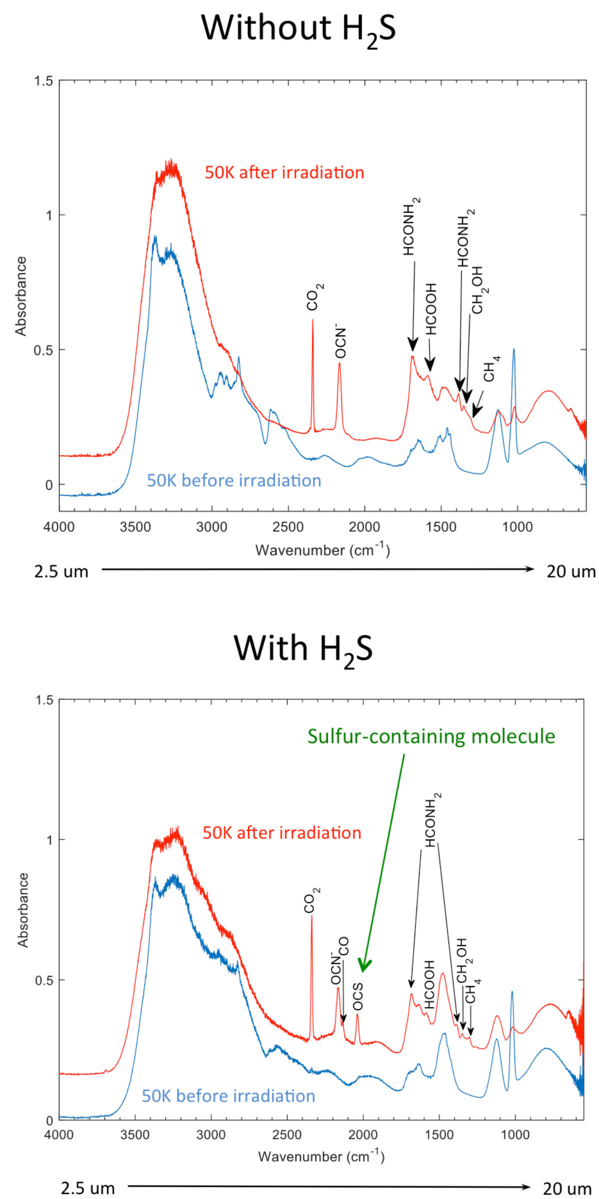

Figure 10. Infrared spectra comparing three and four ice mixtures at 50 K before and after irradiation with 10 KeV electrons and an electron fluence of 2 x 10^{21} eV/cm^2. The primary difference is the formation of OCS in the four ice mixture.

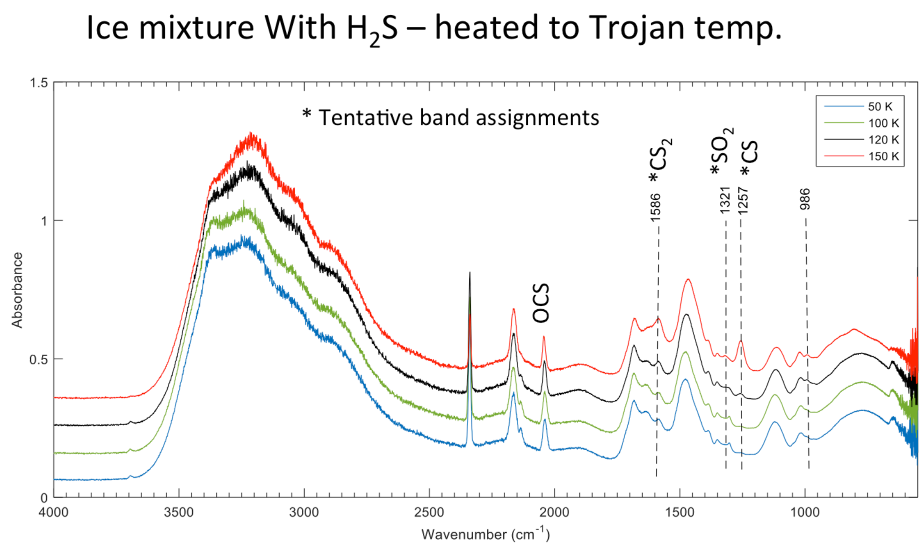

Figure 11. The evolution of sulfur containing species in ices during heating to Trojan temperatures showing the retention of OCS and an increase in CS and SO_2. None of these features are present in the ice mixtures without sulfur, providing confirmation that they are sulfur-associated species.

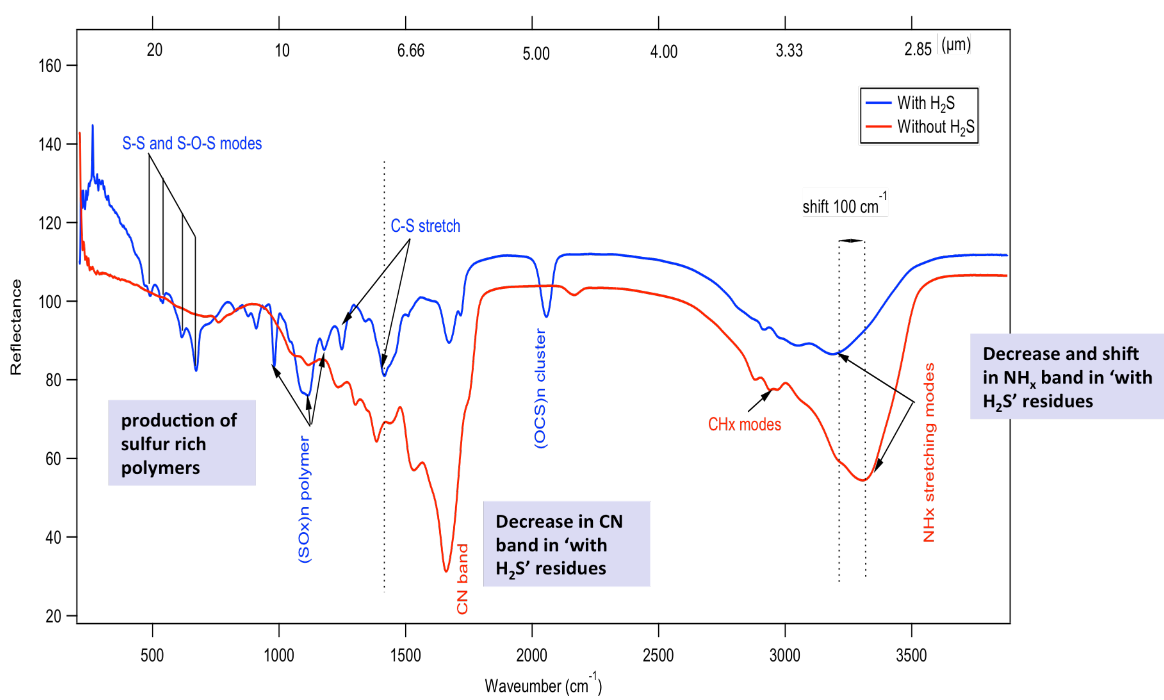

Figure 12. Spectra of non-volatile residues from 3-ice and 4-ice simulants taken at room temperature.

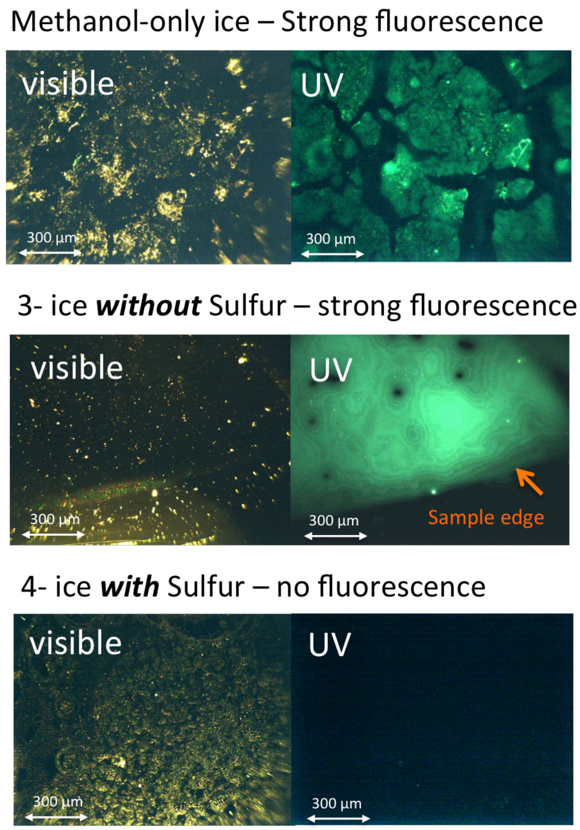

Figure 13. Microscopic images of the residues at room temperature when illuminated with visible light and UV light. A UV filter is used to block reflected UV light, revealing only fluorescence at visible wavelengths. The presence of sulfur creates chemical changes resulting in a complete lack of fluorescence.

Fluorescence

In order to further probe the chemical differences between residues that formed with- and without-H_2S, we observed these samples in a microscope under UV illumination. The results show that fluorescence is strong in these residues, but is notably absent when sulfur is present (see Figure 13). This is indicative of the large chemical changes caused by the presence of sulfur in these residues, as indicated by the differences in the infrared spectra shown in Figure 12. When sulfur is present, it largely dominates the chemistry, limiting the formation of other compounds containing C, O, N, and H.

5.2 Observational Results

Trojan asteroid spectra in the 3 µm region

While the composition of the Trojans has been shown to be similar to comets in terms of silicates using mid-infrared spectra, no other compositional information has yet been reported. In order to further explore the composition of the Trojans and explore their link to Kuiper belt objects, as part of this project we have obtained spectra of eight less-red and eight red Trojans in the 2.2 – 3.8 µm region. This work is reported in detail in Brown, 2016. The signal in this region is particularly weak, and previous attempts have been limited by low signal-to-noise. In this work, using NIRSPEC infrared medium resolution spectrograph at the Keck Observatory, statistically

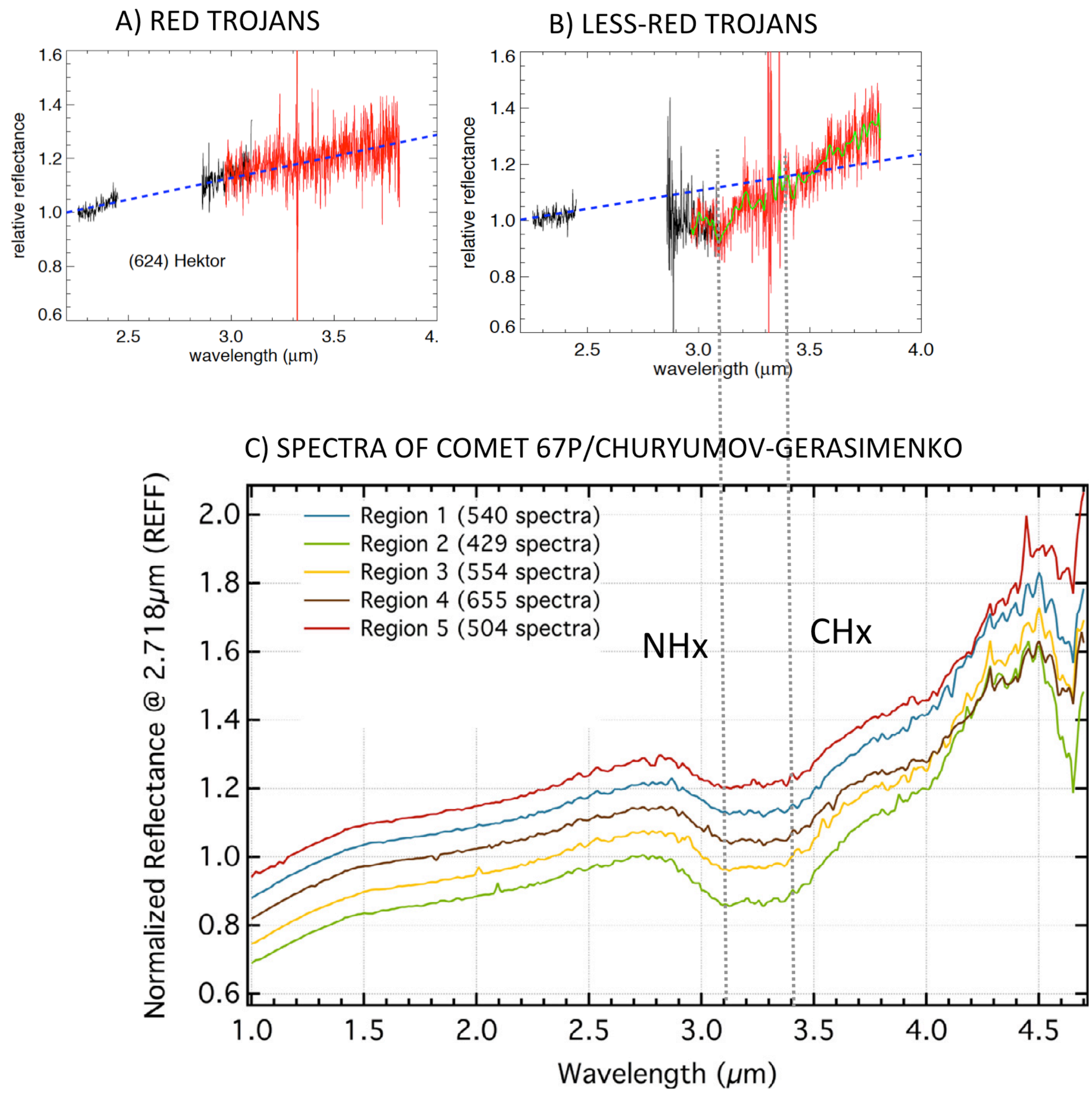

Figure 14. A) Figure from Brown, 2016 showing lack of spectral features in the 3 um region of red Trojans. B) Figure from Brown, 2016 showing an average of spectra from six less-red Trojans with the 3.1 um feature visible. C) VIRTIS/Rosetta spectra (from Quirico *et al.,* 2016) from five regions on the surface of comet 67P, all showing a broad feature in the 3.0 – 3.5 um region. The two peaks near 3.1 um and 3.4 um are attributed to NHx and CHx. The 3.1 um feature is present in both the Trojan and cometary spectra. It is possible that a 3.4 um feature is present in the Trojan data, but is not resolved due to the low signal-to-noise ratio.

significant features were observable in the spectra. In particular, a feature near 3 µm is visible in the less-red spectra, but not in the red spectra (see Figure 14A and B). This supports the idea that there is a compositional difference between the two Trojan color types. The lack of the 3 um feature in the red spectra is also in agreement with the idea that sulfur reduces spectral contrast in this feature. This evidence is however still circumstantial. We look forward to the results of the Lucy mission as well as JWST which are expected to provide much more detailed spectra and compositional data.

Comparisons to comets

It is interesting to compare Trojan spectra in the 3 µm region with those of comets and other solar system bodies that have been hypothesized to come from the same parent source as the

Trojans. Figure 14C shows spectra taken in this region by the VIRTIS instrument on the Rosetta spacecraft. A broad spectral feature appears in the 3 µm region that could plausibly be two overlapping features from NH_x and CH_x. The spectra of less-red Trojans have the 3.1µm feature, but the signal-to-noise ratio is too low to discern whether the 3.4 µm feature is present.

Comparison to laboratory results

When we examine our laboratory results on the 3-ice (without H_2S) residues – our simulants for the less-red Trojans – we see that the 3.1 µm minimum that is apparent in both the Trojan and cometary data is shifted to shorter wavelengths (see Figure 15). The exact nature of these differences is not known, but can potentially be explained by the differences in peak location for different x-values in NH_x. Which one forms predominantly (e.g. NH, NH_2, NH_4) depends on many environmental and processing factors that may differ from the conditions in our lab simulations.

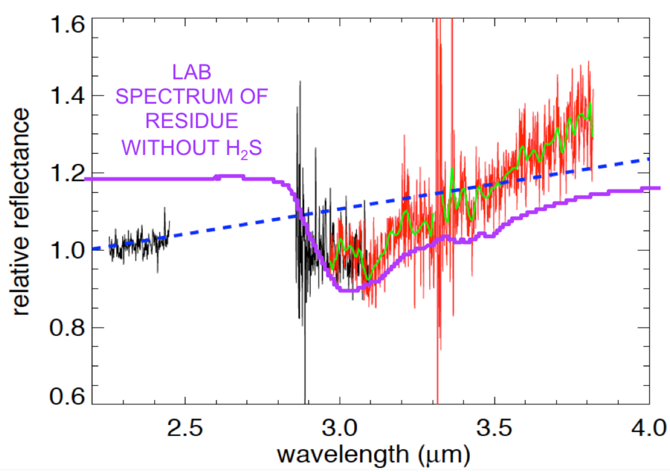

Figure 15. The averaged less-red Trojan spectra from Figure 14B with a room temperature laboratory spectrum from our 3-ice (without H_2S) residue shown in purple.

6 Conclusion

This program set out to bring together a diverse group in order to tackle the challenging goal of testing dynamical models, using the Jupiter Trojan asteroids as a test case. Together we have used theory, laboratory experiments, and telescopic observations to come up with and test a hypothesis that predicts a set of chemical markers of solar system origins. We have fostered a broad collaboration that has contributed in a significant way to the increased interest of the planetary science community in the origins of Trojan asteroids, and to the growing enthusiasm to see a Trojan asteroid mission come to fruition. In this work we have made predictions about the chemistry of the surface of the Trojan asteroids, identifying sulfur as well as N-bearing and other organics as key constituents that can be traced back to their formation processes and dynamical histories. We have presented some supportive evidence for our hypothesis that red and less-red Trojans come from different heliocentric distances in the protoplanetary disk, in the form of laboratory experiments as well as telescopic observations. While we have made significant progress, open questions remain due to the difficulty of remotely obtaining composition and chemistry information from these small, dark targets. We look eagerly to the upcoming Lucy mission and JWST observations to bring more evidence to bear on the problem, hopefully leading to a robust theory of Trojan asteroids origins that can be linked to specific chemical processes such as the ones we propose in this work.

7 PUBLICATIONS

Peer Reviewed Publications

A. Mahjoub, M. Poston, J. Blacksberg, J. Eiler, M.E. Brown, B.L. Ehlmann, K.P. Hand, R. Carlson, M. Choukroun, "Production of sulfur allotropes in electron irradiated Jupiter Trojan ice analogs", submitted to The Astrophysical Journal, May 2017

Brown, M. E., "The 3-4 um spectra of Jupiter Trojan Asteroids", Astronomical Journal, 152(6):159, December 2016

I. Wong and M. Brown, "A Hypothesis For The Color Bimodality Of Jupiter Trojans", Astronomical Journal 152:90 , October 2016

A. Mahjoub, M.J. Poston, K. Hand, M. Brown, R. Hodyss, J. Blacksberg, J., Eiler, R. Carlson, B. Ehlman, M. Choukroun, **"**Electron Irradiation and Thermal Processing of Mixed-ices of Potential Relevance to Jupiter Trojans Asteroids", The Astrophysical Journal, 820:141, April 2016

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9 APPENDIX B: CORE PARTICIPANTS OF THE KISS WORKSHOPS 2012-2013

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