Updating the Results of the Deep Impact Compositional Modeling for Three Other Comet Spectra, YSO HD100546, and the STARDUST PET Findings.

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Background. We have used the infrared mineralogical model derived from the Spitzer IRS observations of the Deep Impact (DI) experiment to study the nature of the dust in the cometary systems 9P/Tempel 1 (T1) [1], C/Hale-Bopp 1995 O1 (HB) [2,3], P/Schwassmann-Wachmann 3 (SW3) [4], and P/Schwassmann-Wachmann 1 (SW1) [5], the YSO HD100546 [3,6], and the debris disk found around the K0V star HD69830 [7,8]. We have found good fits for all of these systems, due to common emission signatures from silicates, water ice, amorphous carbon, and sulfides. There are also major differences - compared to T1, only Mg-rich olivines and little crystalline pyroxenes are found in HB and HD100546. HD100546 lacks amorphous olivine, while being super-rich in amorphous pyroxene. The dust from SW1 and SW3 is much less crystalline, ~30%, is Mg-rich, and does not show strong evidence for phyllosilicates. Located beyond the ice line, SW1 and HB emitted copious amounts of water ice, SW3 at 1.47 AU emitted only water gas. Lacking in carbonaceous and ferrous materials but including small, icy, ephemeral grains, the composition of the HD 69830 dust resembles that of a disrupted P or D-type asteroid.

Achievements of the DI-Spitzer Analysis. The DI-Spitzer analysis has provided a number of important milestones in understanding cometary composition :

-Demonstration that thermal emission from simple randomly oriented fine powder spectra fit the data;

-Definitive detection of PAHs in cometary material;

-Resolution of the question of the "mysterious IR 28 um feature" seen in astronomical sources, to be coming from the ubiquitous sulfides seen in IDPs, in agreement with Keller *et al.* (2002);

- Demonstration that the 6 um complex is due to water gas, and that a substantial amount of the 13- 15 um emission is due to water ice;

-Determination that the interior material of a JFC comet to consist of a large amount of fine grained crystalline silicaceous material, indicative of heavy high-temperature processing;

- Finding that the overall atomic abundance of the most common refractory elements in the solar system comets was solar.

The overall composition of comets presents an interesting puzzle, in that they show clear evidence for materials formed at low temperatures mixed with high temperature materials. Their interiors should be too cold to allow many reactions to progress after formation, yet they have 4.5 Byrs or so for a reaction to run to completion. Broadly, the materials we see dominating in the solid phases are what we would generally expect from thermodynamic processing of the input PSN materials, in agreement with the new STARDUST work [9] when they argue, using atomic and isotopic abundances, for the extensive reworking of the input ISM material into "solar" material incorporated into the comet.

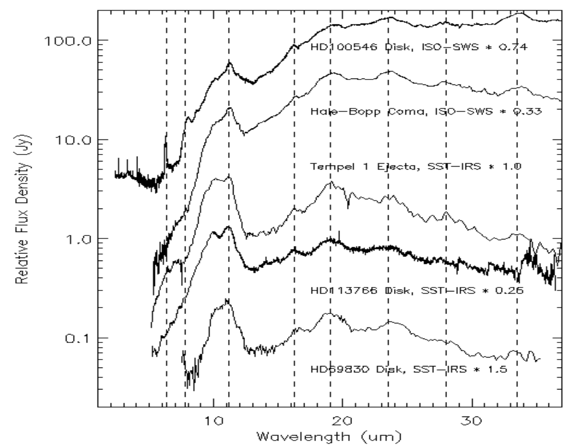

Figure 1 - Mid-IR spectra of YSOs HD100546 and HD113766, comet HB's coma and T1's ejecta, and the asteroidal dust belt of HD69830. Dashed lines are drawn to emphasize common emission features.

Usefulness and Limitations. The new modeling presented here and in [1,3,8] allows us to get beyond the classical olivine-pyroxene-amorphous carbon composition to the second-order, less emissive species like water, sulfides, PAHs, phyllosilicates, and carbonates. On the other hand, there are limitations to the method. There is no petrological or isotopic information, and the results returned are for bulk averages of the observed systems. For example, only very abundant species with strong emission features (>10% of the silicate emission peaks) will be detectable. Alumina (Al_2O_3) and hibonite ($CaAl_2O_6$), extremely stable oxides of aluminum, were not definitively detected in the T1 ejecta even though they are known minor constituents of the pre-solar grain population found in interplanetary dust particles (IDPs). In order to cover the large phase space of of the extreme endstates of each mineral system, and a linear shift in the band positions and strengths between the endstates. E.g., we linearly adjust the balance of forsterite (Fo100, or $MgSi_2O_4$) and fayalite (Fo100, or $Fe_2Si_2O_4$) to fit the observed spectrum, allowing us to determine the total number of each atom present, but cannot distinguish between the presence of Fo50 ($FeMgSi_2O_4$) and a 50-50 mix of (Fo100 + Fa100). The values in the compositional tables should be interpreted in this way. We also cannot distinguish easily between "glassy silicate of non-stoichiometric but near olivine (or pyroxene) composition" and "amorphous silicate of olivine (or pyroxene) composition" and so we assume the presence of stoichiometric glasses when modeling the glassy silicates.

Despite these limitations, at this point in time we are able to determine the overall amounts of the different classes of material (olivines, pyroxenes, sulfides, water, etc.) and the bulk elemental abundances for the most abundant atoms.

Applying the model, with strong checks of its validity, has great potential for interpreting new mid-IR spectra of distant dusty systems like YSOs, debris disks, and PNs.

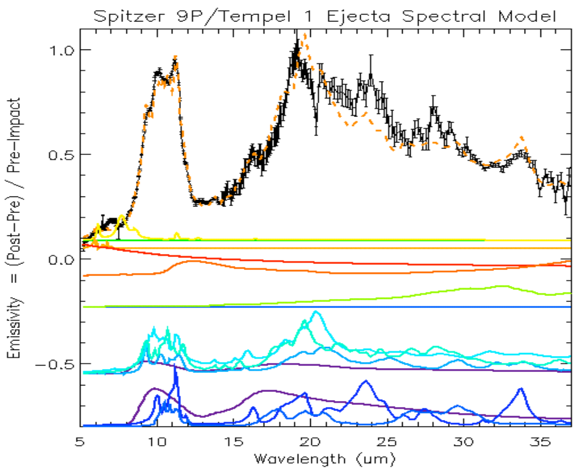

Figure 2 - Best-fit "STARDUST PET" compositional model to the DI-Spitzer observations.

We expect to update the compositional model presented here, with its linear sum of pure mineral end members, by testing, vs. the T1 ejecta emission spectrum, a more precise mineralogical and chemical formulation based on aggregate STARDUST measurements once they are available in the next 3 to 5 years. For example, taking the recently published STARDUST PET results on ~10% of their comet dust sample [9] and creating a bulk compositional model, we can compare it to the DI Spitzer spectrum, to add a measure of "ground truth" to our modeling. Following [1], this is equivalent to taking the best-fit DI model w/o carbonates, phyllosilicates, incorporating FeS and not FeMgS, and restricting the silicates to the Mg-rich olivines, Fe/(Fe+Mg) < 1/3, and the Mg-rich and Ca-rich pyroxenes. The result is a best χ_ν^2 value of 2.55. (recall the 95% C.L. was = 1.13). We can thus easily rule this model out statistically, suggesting a search for alternate answers for the differences in the two compositional models. Note also the poor fits due to lack of emission at 6.5 - 7.5 µm (where carbonates emit), 10 µm (where phyllosilicates emit), 20 - 25 (where Fe rich silicates emit), and 27 - 29 µm (from sulfides).

Possible Reasons for the Differences Between the Two Experimental Outcomes. There are very important systematic effects in both experiments that need to be taken into account when comparing the STARDUST and DI results. Potential issues include the very different nature of the Wild2 and Tempel 1 parent bodies; the high temperatures reached during the STARDUST sample capture, leading to destruction of the sub- 1 um dust particles observed by DI, and deposition of abundant refractory mass along the capture track [9]; chemical processing, including devolatilization and dehydration of cometary surface layers vs. their interiors, so materials like phyllosilicates and carbonates are destroyed and removed from the STARDUST samples; materials created in the puff of hot water vapor created during the DI experiment; the previous impacts near the DI excavation site made these materials by parent body alteration using the hot water vapor evolved; the wrong species has been assigned to for the emission seen in 6.5 - 7.5 and 11-15 um regions, and we need to look for other possibilities (e.g., CH_4, NH_3); poor statistics on the STARDUST sample return, which comprises the total mass equivalent of one 30 um IDP, vs. the few x 10^6 kg observed by DI.

Conclusions. The bottom line is that we need to merge both the DI - Spitzer remote sensing and STARDUST sample return approaches, because the IR spectral modeling has questions of uniqueness, while the in situ sampling technique cannot be applied to distant astronomical sources. Some of this synthesis has already been done in for the DI work, by starting from the best possible candidates for the T1 composition as determined from the IDP, cometary, and astrophysical literature. More work will be done over the next few years to complete this synthesis.

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