DUST AND GAS IN COMET C/2017 K2 (PANSTARRS) WITH JWST.

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Synopsis: Comets, by their journeys into the inner solar system, deliver particulates and volatile gases into their comae that reveal records of the most primitive materials in the solar system. We describe preliminary thermal dust models and volatile gas production rates for dynamically new comet C/2017 K2 (Pan-STARRS, hereafter K2) and share insights into the discovery space that JWST is providing for cometary origins. JWST observed comet K2 through GO 01566 (Woodward PI) using NIRSpec IFU (2.9–5.3µm, $\lambda/\Delta\lambda \approx 1000$) and MIRI IFU (4.9–28.1µm, $\lambda/\Delta\lambda \approx 3000$) at a heliocentric distance of 2.03 au, i.e., at distances where water vapor is the major driver for cometary activity, on 2022 August 21 at JWST distance of 2.34 au (phase angle of 26 degrees). Orbit calculations assign K2 to a long-period and slightly hyperbolic orbit, although K2 may have had an elliptical orbit characteristic of comets in the Oort Cloud family [1, 2]. *Rosetta*'s studies of short period comet 67P/Churyumov-Gerasimenko (67P/C-G) demonstrated that dust-ice particles can be redeposited onto the surface if they not lost from the nucleus' gravitational field and these particles can be re-released into the coma at different parts of the comet's orbit. In contrast, since its discovery at ~16 au, K2 has lost enough mass such that this comet likely is releasing pristine dust and gas into its coma.

Introduction: Cometary dust particles are a crucial component of assessing the physico-chemical conditions in the outer disk out of which they formed. In comparison to the volatiles and organics, the refractory dust particles are more robust and may be traceable to other small bodies. Amorphous silicates (GEMS), abundant in comets [3, 4], appear in Ryugu and the Paris meteorite in regions where aqueous alteration is minimal [5, 6]. When silicate features are identified in cometary IR SEDs, amorphous silicates always are a component and are well-modeled by Mg:Fe=50:50 amorphous olivine and amorphous pyroxene. GEMS can be are associated with D-rich matter or N-rich organics and thereby are traceable to cold cloud conditions [7, 8, 9]; whether GEMS are of interstellar or solar system origin is debated [10, 11]. GEMS appear in *Hyabusa2* carbonaceous asteroid Ryugu and the Paris meteorite in regions where aqueous alteration is minimal [5, 6]. A dark carbonaceous matter also is a ubiquitous component of thermal models for cometary IR SEDs: this component is well-modeled by the optical constants of amorphous carbon [12]. Amorphous carbon is one candidate material for the low albedos of cometary nuclei, with FeS and other carbonaceous materials also being candidates. The nucleus of 67P/C-G has a broad 3.2 µm feature attributed to ammonium salts [13], which are another tracer of cold cloud/disk materials. Ammonium salts are semi-refractory and are not expected to survive in cometary comae. Also on the surface of 67P is an aliphatic carbon '3.4 µm feature' [14], characteristic of meteoritic insoluble organic matter (IOM) [15] and of lines of sight through the warm diffuse ISM [16]. Rosetta's COSIMA mass spectrometer assessed 45wt% of the dust in 67P to be a high molecular weight organic akin to meteoritic IOM, but with less O and more H [17]. For a survey of *Spitzer* comets, thermal models for IR spectra spanning 7–35 µm show that comets contain on average ~55% amorphous carbon [4]. The derived elemental C/Si ratio is closer to the ISM and to solar values and more than ten times greater than elemental C/Si ratios of carbonaceous chondrites [12]. Thus, amorphous silicates, amorphous carbon, ammonium salts, and possibly the organics associated with the dark carbonaceous matter (modeled by amorphous carbon), are thought of as outer disk materials.

As a compliment to these outer disk materials, cometary samples and thermal models for cometary IR spectra reveal Mg-rich crystalline silicates. Mg-rich crystalline olivines (forsterite) and Mg-rich crystalline orthopyroxenes (enstatite ribbons) are the hallmarks of 'hot inner disk condensates' of cometary IR SEDs, chondritic anhydrous IDPs and the least equilibrated carbonaceous chondrites. ^{16}O-enrichments, which were present only in the earliest phases of disk evolution, are correlated with high Mg-contents of Mg:Fe=100:0 — 90:10 [19]. Mg-rich silicate crystals, e.g., LIME olivines, condensed at temperatures ~1800 K [20]. Alternatively, if crystals were Mg:Fe amorphous silicates (perhaps the highly abundant GEMS) that were annealed in shocks near 1100–1200 K then Mg-crystals only could be the result if low oxygen fugacity conditions in the disk allowed Fe-loss following Fe-inter-diffusion [21].

From IR spectroscopy, constraints on the compositions of the olivine crystals yield Mg:Fe=100:0 — 80:20 because the wavelengths of the crystal features are sensitive to Mg:Fe-contents according to laboratory spectra of crystal powders [22, 23]. In contrast to IR spectra, *Stardust* samples reveal a flat distribution of Mg:Fe in the crystalline olivine. Further analyses of the minor elements (Mn, Ca, Cr) in Fe-bearing crystalline olivines in *Stardust* samples and Giant IDPs reveal the Fe-olivines to be mini chondrules [24, 25]. For one such chondrule, ‘Iris’, its age date is >3 Myr after CAI formation [26]. Speaking of igneous particles, Ca,Al-inclusions (CAIs) also are found in *Stardust* samples. One-half of *Stardust* tracks and some IDPs contain “KOOL” particles, which are Ca-Mg-pyroxenes (Kosmochlor pyroxenes Ca- and $NaCrSi_2O_6$-rich clino-pyroxene crystals along with FeO-rich olivine crystals and glass) that formed by igneous or metamorphic processes under high oxygen fugacity. From the spacecraft encounters with 81P/Wild 2 (*Stardust*) and 67P/C-G (*Rosetta*), we know that comets did not form in the outer disk from a homogenized reservoir of materials. Instead, each comet reveals a sampling from the comet-forming regime and of the formation time frames, some of which span ages broader than any one chondritic body. Each comet observed adds important constraints on the radial transport and conditions in the protoplanetary disk and helps to set the context for the materials that are observed to have contributed to other icy bodies (KBOs) and the carbonaceous asteroids such as Ryugu.

JWST Preliminary Results – Comet C/2017 K2: The geocentric-/JWST-distance of the comet allows interesting spatial studies of the inner coma on spatial scales of order 1.5e3 km at superb signal-to-noise ratios. The NIRSpec IFU data reveal in suite of molecular emission lines from the primary species of H_2O through the ‘hot bands’, CO, and CO_2 (only possible from space). Also detected are the important C-bearing gas phase species of CH_4, CH_3OH, and C_2H_6. The OCS band is detected at 4.85 µm and is an important probe of S-chemistry because OCS can be formed by low temperature grain surface reactions of CO with S or possibly by transformation of H_2S, which is abundant in comets, into OCS and S_2 [27]. The $^{13}CO_2$ band also is detected, which can be used to ascertain the optical depth of the $^{12}CO_2$ band, and thus probe conditions in the inner coma of comet K2.

The MIRI IFU data reveals the fundamental water bands and also the CO_2 fundamental band near 15 µm. Spatial distribution studies of the temperature and abundances of the water are facilitated by the high fidelity IFU data. The MIRI IFU IR SED reveals dust thermal emission characterized by a weak silicate feature and a typical comae particle differential size distribution, which translates to abundances of amorphous carbon that are commensurate with other comets [4]. Spectral features of crystalline silicates also are spectrally resolved and their relative strengths assessed. The mineralogy derived from thermal models for the IR dust emission from K2 will be discussed and set into the context of cometary ISM and disk materials [28]. The models for K2 will be compared with *Spitzer* comet survey models [4] to highlight the similarities and differences that are posed by these ground-breaking JWST high fidelity spectra of comet K2.

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