Hapke Modeling of Several KBOs from JWST Observations.

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Introduction: For the last quarter century, spectroscopic studies of Kuiper Belt Objects (KBOs) have been limited to the visible to near-infrared wavelengths ($\lambda <$ 2.5 µm), with some photometric studies of KBOs at $>$ 2.5 µm (e.g., [1, 2]). These observations reveal KBOs are a spectrally diverse population. At visible wavelengths, they have spectral slopes from neutral (~0%/100 nm) to very red (~50%/100 nm) (e.g., [3]). At the near-infrared wavelengths, CH_4, H_2O, C_2H_6, and CH_3OH-ice have been identified on various targets.

With the successful deployment of the James Webb Space Telescope (JWST), we have entered a new era in spectroscopic studies of the Kuiper belt. JWST's NIRSpec (Near Infrared Spectrograph) instrument is capable of obtaining spectra from 0.7 to 5.2 µm in several different spectral settings/resolutions ($\lambda/\Delta\lambda$) from 30 to 3000. We present Hapke analysis of JWST/NIRSpec observations of Quaoar, Gonggong, Salacia, and 2002 MS_4.

Observations: The observations in this work come from two GTO programs. Quaoar (2002 LM_{60}) is a target in GTO program 1254 (P.I. A. Parker). Quaoar was observed (i) with several medium resolution ($\lambda/\Delta\lambda$~1000) gratings covering the 1.0-3.2 µm range and (ii) with the prism mode ($\lambda/\Delta\lambda$~30-300 covering the 0.7-5.2 µm range.). Here we present Quaoar's prism spectrum. We also present data from GTO program 1191 (P.I. J. Stansberry) including NIRSpec/Prism observations of Gonggong (2007 OR_{10}), Salacia (2004 SB_{60}), and 2002 MS_4.

Analysis via Hapke Modeling: We analyze the spectra using Hapke modeling [4, 5]. We calculate the radiance factor of each spectrum generally following the formula:

$$RADF(i,e,g)=\frac{w}{4}\frac{\mu_0}{\mu_0+\mu_e}[(1+B(B_0,h,g))p(g)+H(\mu_0,w)H(\mu_e,w)-1] \qquad (1)$$

Where w is the single scattering albedo, B is the backscatter function which depends on B_0 and h, the amplitude and width of the opposition effect, respectively. The phase function, $p(g)$, assumes the single lobe formalism with asymmetry factor of –0.1. $H(\mu, w)$ is the Chandrasekhar H-function. Finally, μ_0 and μ_e are the cosine of the incidence angle (i) and emergent angle (e) respectively, and g is the phase angle.

Modeling these spectra relies on knowing the optical constants of the refractory materials included in the model. Our models use optical constants of H_2O (crystalline and amorphous), CH_3OH, CO_2, CH_4, C_2H_6, C_3H_8, tholins (P_h from [6]). The optical constants of H_2O and CH_3OH are over a range of temperatures likely found in the Kuiper belt and we apply linear interpolation to use estimates of their optical constants at different temperatures.

We have multiple ways of assuming different arrangements of the surface. These are briefly outlined below:

- Areal Units – A linear combination of Eq 1 weighted by the subtended fractional area.
- Intimate Mixture (type 1) – A mixture of different grains with each grain assumed to be pure. This is sometimes referred to as a "salt-and-pepper" mixture.
- Intimate Mixture (type 2) – A grain is composed of the host material with some fraction of inclusions from another. The optical constants for both species are combined following Maxwell Garnett theory.
- Two Layers – A layer of one species or mixture is overlaid with another.
- Small grains – When the size parameter, $2\pi d/\lambda << 1$ (where d is the grain diameter and λ is the wavelength), Mie scattering is accounted for. At these wavelengths, d is typically < 1 µm.

Prism spectra of **Salacia & 2002 MS_4** are shown in Figs 1 & 2. These spectra show absorption due to H_2O-ice at 1.5, 1.65, 2.0, and 3.0 µm. The spectra also have strong Fresnel peaks around 3.1 µm also due to crystalline H_2O-ice. Also noted in these spectra is a feature at 4.25 µm attributed to CO_2-ice. Our modeling suggests (i) some of the CO_2-ice has sub-micron grain size (ii) amorphous H_2O-ice is present, and (iii) the surface temperature is about 30 K and 65 K for Salacia and 2002 MS_4, respectively.

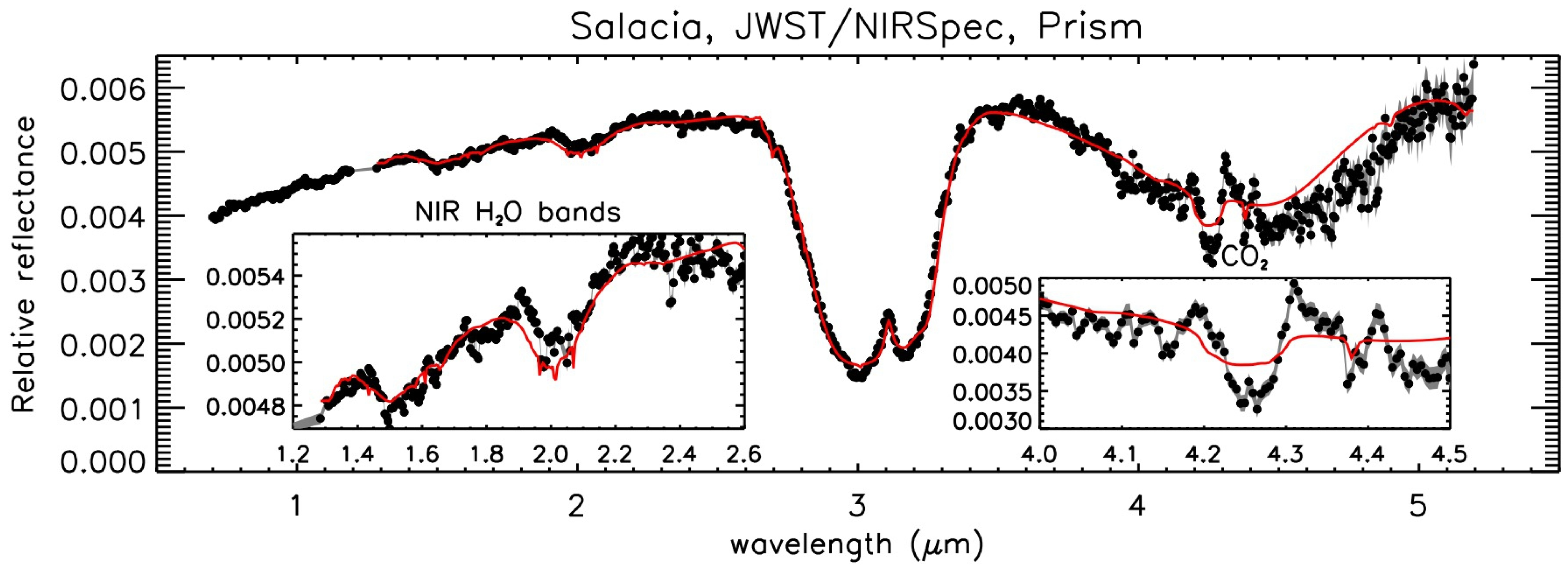
Salacia (T = 30 K)		
Areal Unit 1 (40.8%) – intimate mix (type 1)		
P_h	79.8%	d=8.2 µm
Cryst H_2O	8.9%	d=1.3 µm
Amor H_2O	9.4%	d=1.1 µm
CO_2	1.8%	d=1.0 µm
Areal Unit 2 (38.6%)		
Cryst H_2O	100%	d=182 mm
Areal Unit 3 (20.5%) – two layers, τ_0 = 0.0124 (top layer)		
CO_2 (bottom)	100%	d=33 µm
CO_2 (top)	100%	d=0.12 µm

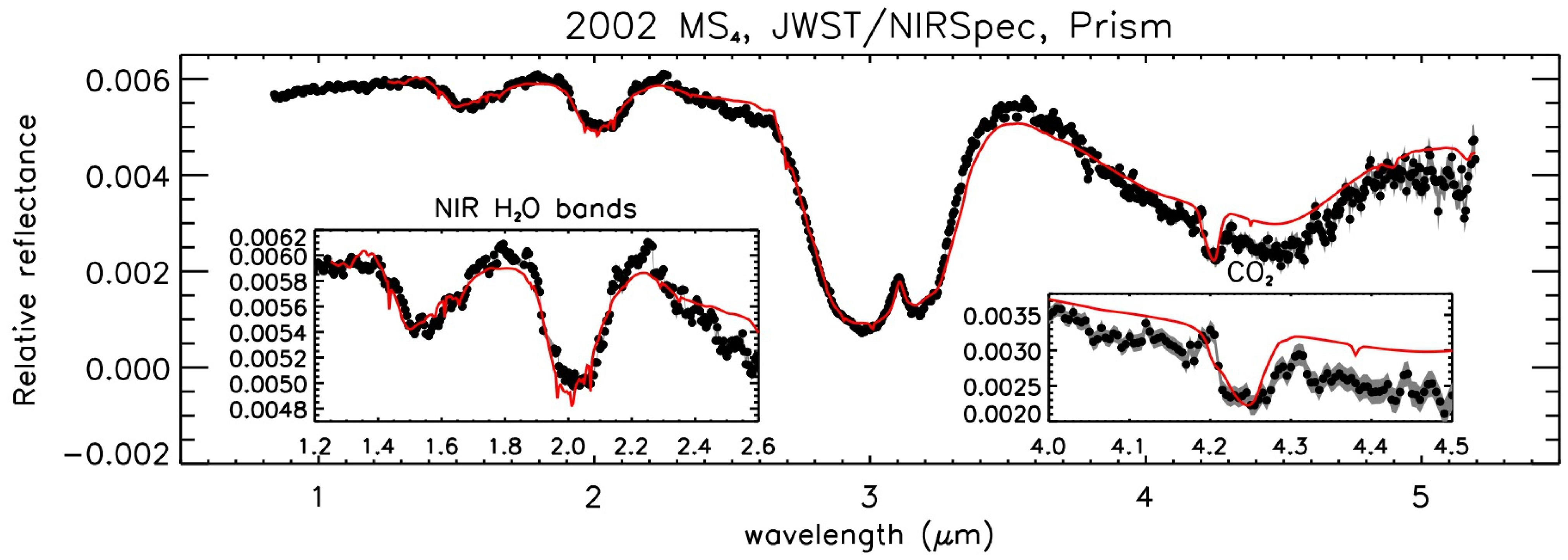
2002 MS_4 (T = 65 K)		
Areal Unit 1 (28.9%) – intimate mix (type 1)		
P_h	43.4%	d=54 µm
Cryst H_2O	12.0%	d=1.3 µm
Amor H_2O	34.8%	d=1.1 µm
CO_2	9.81%	d=49 nm
Areal Unit 2 (30.4%)		
Cryst H_2O	100%	d=697 mm
Areal Unit 3 (40.7%) – two layers, τ_0= 0.0148 (top layer)		
CO_2 (bottom)	100%	d=49 µm
CO_2 (top)	100%	d=20 nm

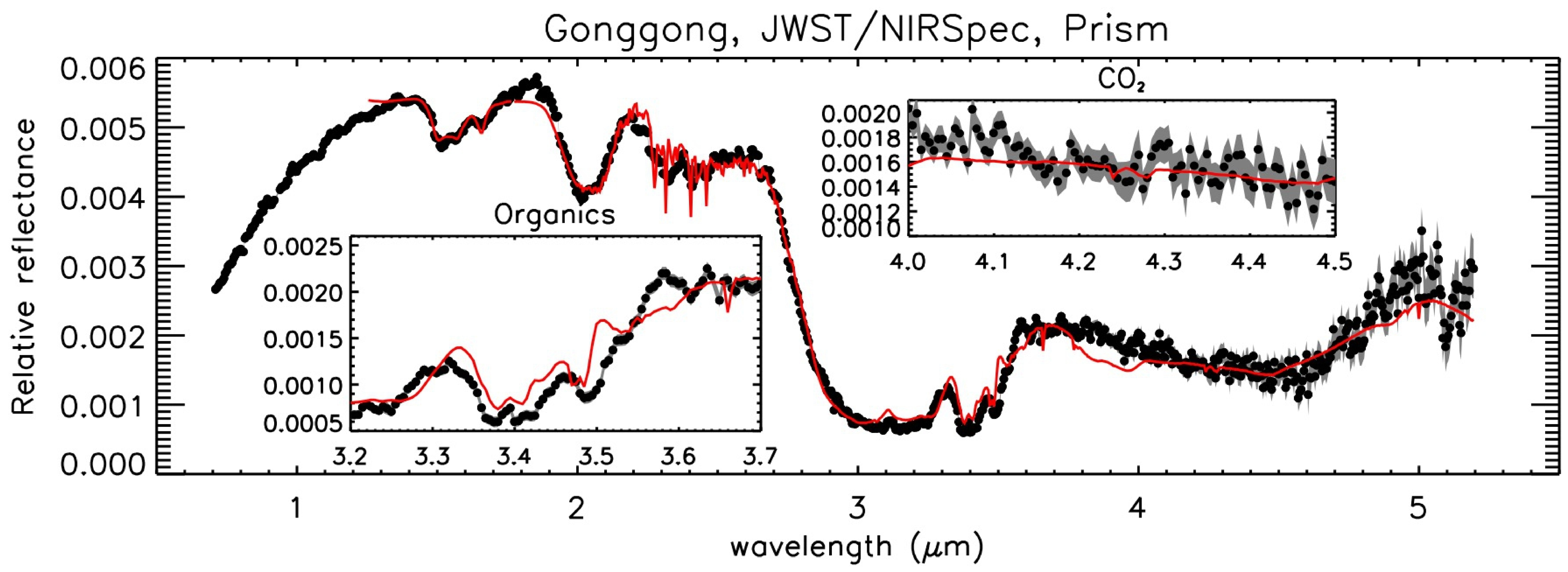
Prism spectra of **Gonggong & Quaoar** are shown in Figs 3 & 4. These spectra show absorption due to H_2O-ice at 1.5, 1.65, 2.0, and 3.0 µm. The spectra have weak Fresnel peaks around 3.1 um compared to the same features in the spectra of Salacia and 2002 MS_4. We also see absorption from 3.35-3.55 µm commonly attributed to organics. Our best fitting models suggest this band is due to a combination of C_2H_6, C_3H_8, and CH_3OH-ice. Other hydrocarbons are plausible, but optical constants are not always available. Absorption due to CO_2-ice is not detected on Gonggong, but a weak feature is seen on Quaoar, but its position and shape are different from those seen on Salacia or 2002 MS_4. While CO_2-ice is included in the Quoaor model, its is difficult for us to fit because the model rejects its presence.

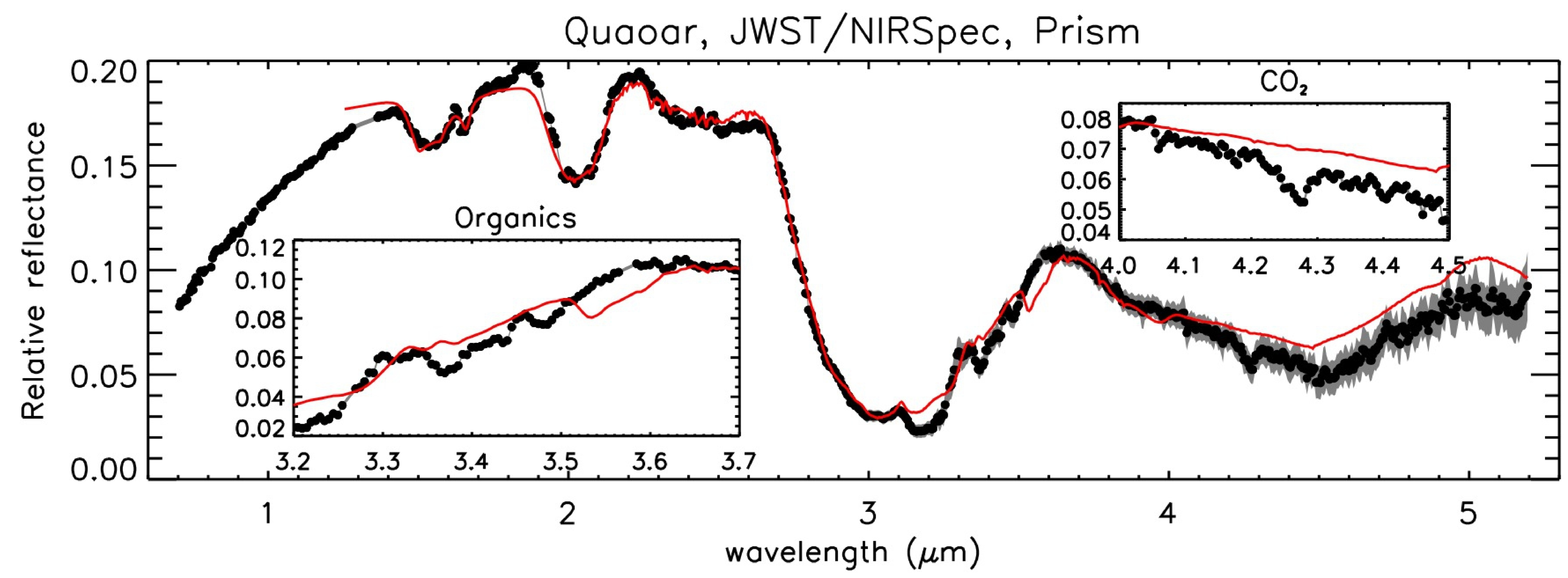
Gonggong (T = 65 K)		
Areal Unit 1 (99.5%) – intimate mix (type 1)		
P_h	99.6%	d=14.4 mm
Cryst H_2O	<<0.01%	d=25.8 µm
Amor H_2O	0.3%	d=5.1 µm
Areal Unit 2 (0.4%)		
Cryst H_2O	100%	d=190 mm
Areal Unit 3 (0.1%) – two layers w/intimate mix (type 1), τ_0= 0.0124 (top layer)		
P_h (bottom)	22.3%	d=1.0 µm
Cryst H_2O (bottom)	66.0%	d=6.1 µm
C_2H_6(bottom)	7.0%	d=3.5 µm
C_3H_8 (bottom)	4.6%	d=1.2 µm
CH_3OH (top)	100%	d=5.7 µm

Quaoar (T = 55 K)		
Areal Unit 1 (29.9%) – intimate mix (type 1)		
P_h	22.2%	13.4 µm
Cryst H_2O	0.1%	102 µm
Amor H_2O	77.6%	8.8 µm
Areal Unit 2 (60.8%)		
Cryst H_2O	100%	1.4 mm
Areal Unit 3 (9.3%) – two layers w/intimate mix (type 1), τ_0 = 0.274 (top layer)		
P_h (bottom)	27.9%	8.1 µm
Cryst H_2O (bottom)	70.4%	6.9 µm
C_2H_6 (bottom)	1.7%	20.1 µm
C_3H_8 (top)	48.2%	27.8 µm
CH_3OH (top)	51.8%	3.0 µm
Areal Unit 4 (0.01%) – two layers w/intimate mix (type 1), τ_0 = 0.0273 (top layer)		
P_h (bottom)	100%	0.6 µm
CO_2 (top)	26.6%	3.4 µm
Cryst H_2O (top)	73.3%	693 µm









Figures 1-4: JWST/NIRSpec Prism spectra of Salacia, 2002 MS_4, Gonggong, and Quaoar (from top to bottom). The data are shown as black points, with uncertainties as the grey cloud. Our best fit Hapke models (fit from 1.25 to 5.2 µm) are shown in red. Insets show different regions of spectral interest such as the near-infrared H_2O-ice bands from 1.25 to 2.5 µm, the organics band around 3.4 µm, and the CO_2 band around 4.25 µm.

Conclusion & Future Work: Crystalline H_2O-ice is detected on all four objects examined here, although modeling does suggest amorphous H_2O is also present. CO_2-ice is detected on two, possibly three, of the targets, although the position and shape of the band on Quaoar is different from Salacia and 2002 MS_4. No CO_2-ice is noted in the spectrum of Gonggong. We detect organics which our models suggest is a combination of at least C_2H_6, C_3H_8, and CH_3OH. Other hydrocarbons are possible, but we lack high quality optical constants. In the future we will develop models to include the 0.7-1.25 µm range and CH_4-ice where organics are seen.

References: [1] Emery, J. P., et al. (2007) vol. 39 of AAS/Division for Planetary Sciences Meeting Abstracts 49.08. [2] Fernández-Valenzuela, E., et al. (2021) Planet. Sci. J 2(1):10.arXiv:2011.07121. [3] Hainaut, O. R., et al. (2012) A&A 546:A115.ArXiv:1209.1896. [4] Hapke, B. (1993) Theory of reflectance and emittance spectroscopy. [5] Hapke, B. (2012) Theory of Reflectance and Emittance Spectroscopy. [6] Jovanović, L., et al. (2021) Icarus 362:114398.