Measurements of Coma Physics and Ice Composition in Comet D/2012 S1 (ISON) to Small Heliocentric Distances as Revealed at Infrared Wavelengths. M. A. DiSanti[1,2], B. P. Bonev[1,3], E. L. Gibb[1,4], L. Paganini[1,3], G. L. Villanueva[1,3], M. J. Mumma[1,2], J. V. Keane[5], G. A. Blake[1,6], N. Dello Russo[7], K. J. Meech[5], R. J. Vervack, Jr.[7], A. J. McKay[8] [1]Goddard Center for Astrobiology, NASA-Goddard Space Flight Center, Greenbelt, MD, USA (michael.a.disanti@nasa.gov), Solar System Exploration Division, Code 690, NASA-Goddard Space Flight Center, Greenbelt, MD, [3]Department of Physics, The Catholic University of America, Washington, DC, [4]Department of Physics and Astronomy, University of Missouri-St. Louis, Saint Louis, MO, [5]Institute for Astronomy, University of Hawai'i at Manoa, Honolulu, HI, [6]Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, CA, [7]The Johns Hopkins University Applied Physics Laboratory, Laurel, MD 20723-6099, [8]University of Texas-Austin/McDonald Observatory, Austin, TX

Introduction: The apparition of dynamically new, Sun-grazing Comet C/2012 S1 (ISON) [1] afforded a rare opportunity to conduct serial studies over a large range of heliocentric distances (R_h), and in particular to well within 1 AU. As part of a coordinated world- and solar system-wide observing campaign, we report production rates for H_2O and eight trace molecules (CO, C_2H_6, CH_4, CH_3OH, NH_3, H_2CO, HCN, C_2H_2) using the high-resolution spectrographs NIRSPEC [2] at Keck 2 and CSHELL [3] at the NASA-IRTF on ten pre-perihelion dates encompassing R_h = 1.213 – 0.344 AU. Significant studies that emerged include spatially resolved measurements of H_2O excitation in the coma [4, 5], a 3σ upper limit for HDO/H_2O of 2.0 VSMOW [6], and serial measurements of H_2O production and of molecular abundance ratios as functions of R_h [5, 7].

Spatially Resolved Excitation of H_2O: The rotational temperature (T_{rot}) of water was measured along the slit (Fig. 1). This study revealed that elevated values of T_{rot} persisted to beyond 1000 km from the nucleus, above those expected if adiabatic cooling dominated excitation conditions in the coma. This work is driving physical coma models [8], which in turn provide synergy with observations.

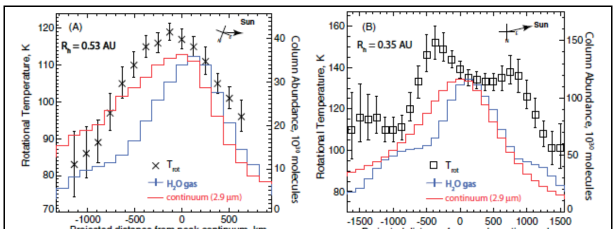

Figure 1. Spatially resolved measurements of dust continuum and gaseous H_2O emission intensities, together with T_{rot} of H_2O along the CSHELL slit, which was oriented with respect to the projected sunward direction as shown in each panel, on (A) UT November 17.73 and (B) November 22.74. Respective R_h-values are also indicated.

Production Rates and Molecular Abundances:

Water Production Rates. Thirty-two measurements spanned two orders of magnitude (Fig. 2). We found a long-term heliocentric dependence consistent with $Q(H_2O) = (1.89 \pm 0.11) \times 10^{28} R_h^{(-3.10\pm0.09)}$, based on 25 of these that we take to represent "baseline" measurements of water production in Comet ISON.

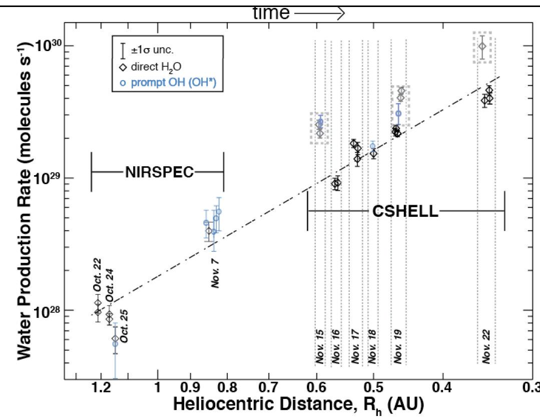

Figure 2. Evolution of water production in Comet ISON spanning 2013 October 22 through November 22. The NIRSPEC results were obtained simultaneously on each date; the points on November 7 are separated horizontally only to visualize them more clearly. Of the 32 measurements, seven (in dashed boxes) were associated with periods of enhanced water production (i.e., with "outbursts"). A heliocentric fit (dot-dashed line) excluding these seven points resulted in a power law steeper than the canonical insolation-limited R_h^{-2} slope.

Molecular Abundance Ratios. Abundances of CO, C_2H_6, and CH_4 with respect to H_2O were relatively constant with R_h, and were below their corresponding mean values measured among a dominant sample of Oort cloud comets. CH_3OH was also depleted for R_h > 0.5 AU, but was closer to its mean value for $R_h \leq 0.5$ AU. The remaining four molecules exhibited higher abundance ratios within 0.5 AU: for R_h > 0.8 AU, NH_3 and C_2H_2 were consistent with their mean values while H_2CO and HCN were depleted. For R_h < 0.5 AU all four were enriched, with NH_3, H_2CO, and HCN increasing most (Fig. 3, Table 1).

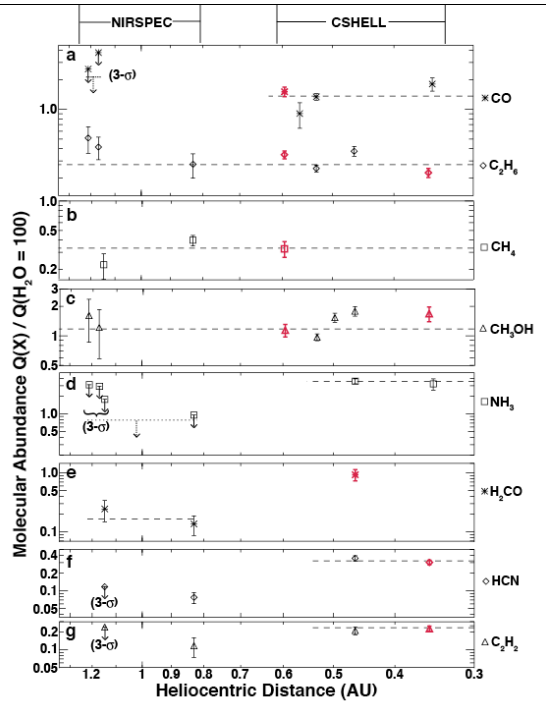

Figure 3. Evolution of abundance ratios relative to H_2O in Comet ISON, with molecules listed at right. Points shown in red were measured during periods of enhanced gas production (i.e., during "outburst"). No discernable dependence of composition on "baseline" versus "outburst" activity was seen.

Table 1. Abundances in ISON compared to other comets and interstellar sources

	CO	C_2H_6	CH_4	CH_3OH	NH_3	H_2CO	HCN	C_2H_2
ISON [a]								
$R_h > 0.5$ AU [a]	1.3 ± 0.1	0.28 ± 0.02	0.33 ± 0.03	1.1 ± 0.1	< 0.78	0.16 ± 0.05	0.07 ± 0.02	0.11 ± 0.04
$R_h < 0.5$ AU [a]	1.8 ± 0.4	0.26 ± 0.02	----------	1.7 ± 0.2	3.5 ± 0.3	0.91 ± 0.20	0.32 ± 0.02	0.24 ± 0.02
"Normal" [b]	{4.0}	0.62 ± 0.02	{0.87}	2.2 ± 0.2	0.75 ± 0.23	{0.25}	0.18 ± 0.03	0.11 ± 0.02
73P/S-W3-C [c]	0.50 ± 0.13 [d]	0.15 ± 0.04 [e,f]	< 0.25 [f]	0.14 ± 0.02 [f]	< 0.3 [f]	0.11 ± 0.02 [f]	0.18 ± 0.02 [f]	< 0.033 [f]
C/1999 S4 [c]	0.9 ± 0.3 [g]	0.11 ± 0.02 [g]	0.12 ± 0.02 [g]	< 0.26 [g]	----------	----------	0.10 ± 0.03 [g]	< 0.14 [h]
C/2001 A2 [h]	3.9 ± 1.1	1.70 ± 0.20	1.2 ± 0.2	3.0 ± 0.4	1.38 ± 0.37	0.24 ± 0.05	0.6 ± 0.1	0.5 ± 0.1
Low-mass [i]	29	----------	5	3	5	----------	0.3	----------
High-mass [i]	13	----------	2	4	5	----------	0.6	----------

[a] This work. Mean molecular abundance ratios relative to H_2O (in percent) in Comet ISON are listed separately for $R_h > 0.5$ and $R_h < 0.5$ AU, excluding upper limits except for cases in which only these were obtained (i.e., NH_3 for $R_h > 0.5$ AU). Values in red, black, and blue indicate "organics-depleted," "organics-normal," and "organics-enriched," respectively, as defined by the current compositional taxonomy.

[b] "Normal" refers to a sample of 12 comets in which C_2H_6 was measured, all of which come from the Oort cloud, excepting the compositional measurement of the ejecta from Jupiter family Comet 9P/Tempel 1 (Mumma et al. 2005, *Science*, **310**, 270) resulting from the Deep Impact experiment. Values for CH_3OH, HCN, and C_2H_2 draw on a subset of these: CH_3OH and HCN, 11 comets; C_2H_2, 9 comets. For CO, CH_4, and H_2CO median values are listed since these molecules show larger variations among comets measured to date (both from Oort cloud and Jupiter family populations), by factors of 10 or more. The mean value listed for NH_3 is based on 12 comets, six of which are in the C_2H_6 group and all excepting 6P/d'Arrest (Dello Russo et al. 2009, *Astrophys J*, **703**, 187) are from the Oort cloud. For all molecules, upper limits are excluded when calculating "normal" (current mean or median) values.

[c] Comets 73P/Schwassmann-Wachmann 3 and C/1999 S4 (LINEAR) are classified "organics-depleted."

[d] DiSanti et al. (2007), *Astrophys J (Lett)*, **661**, L101.

[e] Villanueva et al. (2006), *Astrophys J (Lett)*, **650**, L87.

[f] Dello Russo et al. (2007), *Nature*, **448**, 172.

[g] Mumma et al. (2001), *Science*, **292**, 1334.

[h] C/2001 A2 (LINEAR) is classified "organics-enriched." Values are taken from Magee-Sauer (2008, *Icarus*, **194**, 347) at R_h = 1.2 AU. H_2CO changed from 0.89% to 0.21% on successive dates at 1.2 AU and an abundance for CH_4 as high as 3.5% (dependent on the value for T_{rot} used) was reported at R_h = 1.6 AU (Gibb et al. 2007, *Icarus*, **188**, 224), suggesting chemical heterogeneity in the nucleus.

[i] "Low-mass" and "high-mass" refer to proto-stellar sources observed by the Spitzer survey; median ice abundances (relative to H_2O = 100) are taken from Öberg et al. (2010, *Astrophys J*, **716** 825) and Gibb et al. (2004, *Astrophys J Supp*, **151**, 35).

References: [1] Nevski V. and Novichonok A. (2012) *CBET 3238*. [2] McLean I. S. et al. (1998) *SPIE 3354,* 566-578. [3] Tokunaga A. et al. (1990) *SPIE 1235,* 131-143. [4] Bonev B. P. et al. (2014) *Astrophys. J. Lett. 796,* L6 (6pp). [5] Dello Russo N. et al. (2016) *Icarus 266*, 152-172. [6] Gibb E. L. et al. (2016) *Astrophys. J.,* in press. [7] DiSanti M. A. et al. (2016) *Astrophys. J.,* in press. [8] Fougere N. et al. (2014) *BAAS 46*, id#113.03 (DPS meeting #46).

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