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Supporting Information for

The Composition of 96 keV W^+ in Saturn's Magnetosphere

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Contents of this file

Table S1. Molecular Ionic Radius and Diameter Information

		Radius, r_I		Diameter		Reference
H_3O^+	hydroxonium (hydronium)	0.100 nm	= 100.0 pm	0.200 nm	= 200.0 pm	(MCa;Marcus, 2012)
H_2O^+	water ion	0.138 nm	= 138.0 pm	0.276 nm	= 276.0 pm	(MCa)
H_2O^o	water(diameter)	1.38 Å	= 138.0 pm	2.75 Å	= 275.0 pm	(MCc)
OH^+	hydroxyl	1.032 Å	= 103.2 pm	2.064 Å	= 206.4 pm	(NIST)
OH^-	r_{OH-} (r_{OHo} ± 0.002 A)		= 103.7 pm		= 207.4 pm	(Branscomb, 1966)
OH^-	hydroxide	0.970 Å	= 97.0 pm	1.94 Å	= 194.0 pm	(NIST)
OH^-		0.110 nm	= 110.0 pm	0.220 nm	= 220.0 pm	(MCb)
OH^o	hydroxyl radical		= 103.5 pm		= 207.0 pm	(average: OH^+,OH^-)
O^o	oxygen atom	60pm	= 60.0 pm		= 120.0 pm	(Slater, 1964)

References:

Chaplin, M. (2019), Water Structure and Science, London South Bank University (http://www1.lsbu.ac.uk/water/water_structure_science.html).
MCa: Chaplin19a: http://www1.lsbu.ac.uk/water/hydrogen_ions.html
MCa: "H_3O^+ has an effective ion radius of 0.100 nm, ... less than that of the H_2O molecular radius (0.138 nm)."
MCb: Chaplin19b: http://www1.lsbu.ac.uk/water/ionisoh.html
MCc: http://www1.lsbu.ac.uk/water/water_molecule.html

Marcus, Y. (2012). Volumes of aqueous hydrogen and hydroxide ions at 0 to 200 °C. *Journal of Chemical Physics, 137*, 15, 154501-254501-5. https://doi.org/10.1063/1.4758071

Branscomb, L. M., (1966). Photodetachment cross section, electron affinity, and structure of the negative hydroxyl ion. *Physical Review, 148*, 1, 11-18. https://org/doi/10.1103/PhysRev.148.11

Slater, J. C., (1964). Atomic Radii in Crystals. *Journal of Chemical Physics, 41*, 10, 3199-3204. https://org/doi/10.1063/1.1725697

Figure 4 of Cassidy & Johnson (2010): neutral density at Rhea's orbital distance

(a)	O-density(at Rhea) ~70/cc		(b)	OH-density(at Rhea) ~20/cc	
(a)	$r_I+r_N(O\_H_2O^+)$	= (138+60)e-12 = 198e-12	(b)	$r_I+r_N\ (OH\_H_2O^+)$	= (138+97)e-12 = 235e-12
	$(r_{I+}r_N)^2\ N_N$	= (198e-12 m)^2 x 70/cc		$(r_{I+}r_N)^2\ N_N$	= (235e-12 m)^2 x 20/cc
→→	$(r_{I+}r_N)^2\ N_N$	= 2.7e-18	→→	$(r_{I+}r_N)^2\ N_N$	= 1.1e-18

Figure 6 of Smith et al. (2010): neutral density at Rhea's orbital distance, average of Cassini E3 and E5 flybys

(c)	O-density(at Rhea) ~100/cc		(d)	OH-density(at Rhea) ~50/cc	
(c)	$r_I+r_N(O\_H_2O^+)$	= (138+60)e-12 = 198e-12	(d)	$r_I+r_N(O\_H_2O^+)$	= 138+97 = 235e-12
	$(r_{I+}r_N)^2\ N_N$	= (198e-12 m)^2 x 100/cc		$(r_{I+}r_N)^2\ N_N$	= (235e-12 m)^2 x 50/cc
→→	$(r_{I+}r_N)^2\ N_N$	= 3.9e-18	→→	$(r_{I+}r_N)^2\ N_N$	= 2.8e-18

Table S2. Grain Size and Density Information

Srama et al. (2011): give $n(r) = 20(r - 2.8)^{-4.6}$ for grain density falloff (best fit at 3.95-8.73 R_s)
Enceladus: $20\ (3.95 - 2.8)^{-4.6} = 10.515258 : 10.5$
Rhea: $20\ (8.73 - 2.8)^{-4.6} = 0.005559. : 5.56e\text{-}3$
Grain/dust density scale factor: $0.005559/10.515258 = 0.000529 \sim 5e\text{-}4$
(e) grain size = 1.0 nm = 0.3e-9 = 1000e-12 m, from Fig.10, Dong et al. (2015)
(f) grain size = 2.0 nm = 2.0e-9 = 2000e-12 m, from Fig.10, Dong et al. (2015)
grain density@Rhea = 2000 x 5e-4 = 1, from Fig.11a, Dong et al. (2015); Fig.11,Srama et al. (2011)
(e) 1.0 nm grains: $r_I + r_G = 138 + 1000 = 1138e\text{-}12$
$(r_I + r_G)^2 N_{G(1)} = (1138e\text{-}12)^2 * 2000 * (1) * 5e\text{-}4$
→→ $(r_I + r_G)^2 N_{G(1)} = 1.3e\text{-}18$
(f) 2.0 nm grains: $r_I + r_G = 138 + 2000 = 2138e\text{-}12$
$(r_I + r_G)^2 N_{G(2)} = (2138e\text{-}12)^2 * 1000 * (1) * 5e\text{-}4$
→→ $(r_I + r_G)^2 N_{G(2)} = 2.3e\text{-}18$
(g) 4.0 nm grains: $r_I + r_G = 138 + 4000 = 4138e\text{-}12$
$(r_I + r_G)\ N_{G(4)} = (4138e\text{-}12)^2 * 200 * (1) * 5e\text{-}4$
→→ $(r_I + r_G)\ N_{G(4)} = 1.7e\text{-}18$

Table S3. Mean Free Path Ratio ($\Gamma_{N:G}$) Calculations for H_2O^+ in neutral gas (a-d) and grains (e,f) †

--------(*::e, 1 nm)----------	--------(*::f, 2 nm)----------	--------(*::g, 4 nm)----------
a: 1.3e-18/2.7e-18 = 4.81e-1	a: 2.3e-18/2.7e-18 = 8.52e-1	a: 1.7e-18/2.7e-18 = 6.29e-1
b: 1.3e-18/1.1e-18 = 1.18e0	b: 2.3e-18/1.1e-18 = 2.09e0	b: 1.7e-18/1.1e-18 = 1.55e0
c: 1.3e-18/3.9e-18 = 3.33e-1	a: 2.3e-18/3.9e-18 = 5.90e-1	a: 1.7e-18/3.9e-18 = 4.36e-1
d: 1.3e-18/2.8e-18 = 4.64e-1	b: 2.3e-18/2.8e-18 = 8.21e-1	b: 1.7e-18/2.8e-18 = 6.07e-1

or roughly,

a: [O] ~ [1 nm] ~ 0.48 ~ 1/2	a: [O] ~ [2 nm] ~ 0.85 ~ 1	a: [O] ~ [4 nm] ~ 0.63 ~ 1/2
b: [OH] ~ [1 nm] ~ 1.2 ~ 1	b: [OH] ~ [2 nm] ~ 2 ~ 2	b: [OH] ~ [4 nm] ~ 1.6 ~ 1 1/2
c: [O] ~ [1 nm] ~ 0.33 ~ 1/3	c: [O] ~ [2 nm] ~ 0.6 ~ 1/2	c: [O] ~ [4 nm] ~ 0.44 ~ 1/2
d: [OH] ~ [1 nm] ~ 0.46 ~ 1/2	d: [OH] ~ [2 nm] ~ 0.8 ~ 1	d: [OH] ~ [4 nm] ~ 0.61 ~ 1/2

† https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Book%3A_Thermodynamics_and_Chemical_Equilibrium_(Ellgen)/04%3A_The_Distribution_of_Gas_Velocities/4.12%3A_The_Frequency_of_Collisions_between_Unlike_Gas_Molecules

Sample Calculation for a::e at Rhea:

$A_N = (198e\text{-}12\ m)^2$ $A_G = (1138e\text{-}12\ m)^2$
$N_N = 70/cc$ $N_G = 2000 * 5e\text{-}4$

$$\Gamma_{N:G} = \frac{N_G \times A_G}{N_N \times A_N} = \frac{2000 \times 5e\text{-}4 \times (1138e\text{-}12\ m)^2}{70. \times (198e\text{-}12\ m)^2} = \frac{1.295e\text{-}18}{2.744e\text{-}18} \sim \frac{1.3}{2.7} = 0.48$$

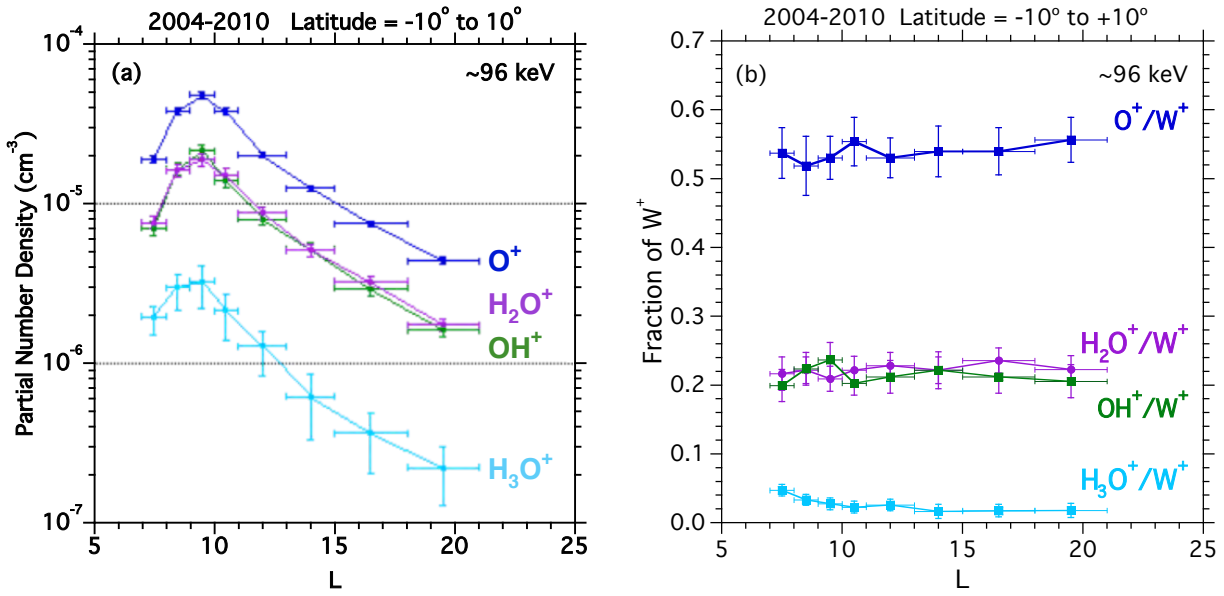

Figure S1 (see Figure 4). (a) The partial number density of energetic, ~96 keV, water group components versus L. (b) The fractional abundance of ~96 keV water group components plotted linearly versus L. The error bars of O^+, OH^+, and H_2O^+ represent the statistical uncertainties from the best fit. The error bars of H_3O^+ represent the spread of values from our three different fits (see text).

Figure S2. Figure 5 from Paranicas et al. (2008)

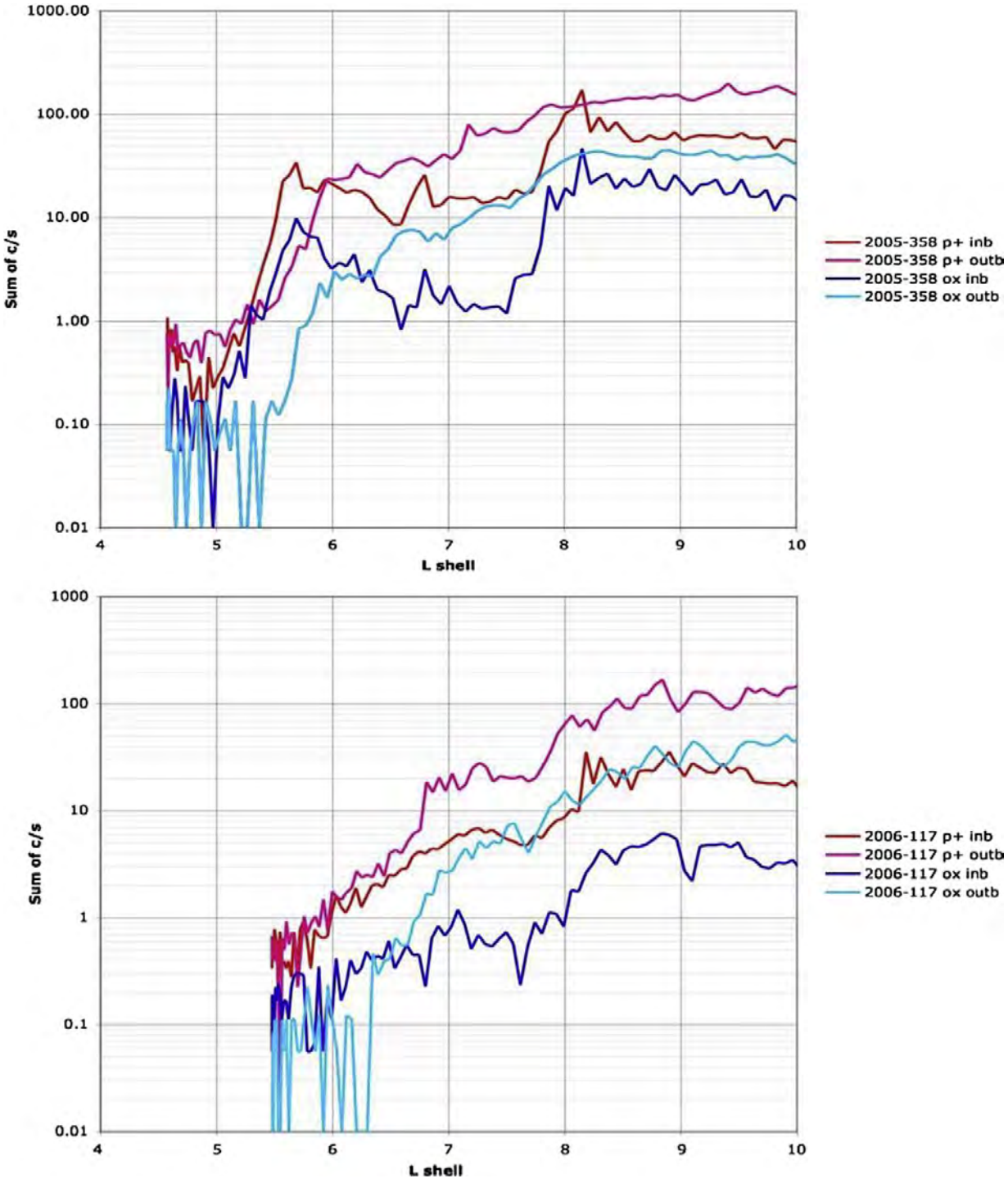

Fig. 5. Summed count rates for the periods in Fig. 3 (top) and Fig. 4 (bottom). The inbound and outbound data are plotted separately with the proton sum red and the oxygen sum blue. The proton (oxygen) sum is over the CHEMS energy range 3–220 (8–220) keV.

Figure S3. Figure 1 from Kollmann et al. (2011)

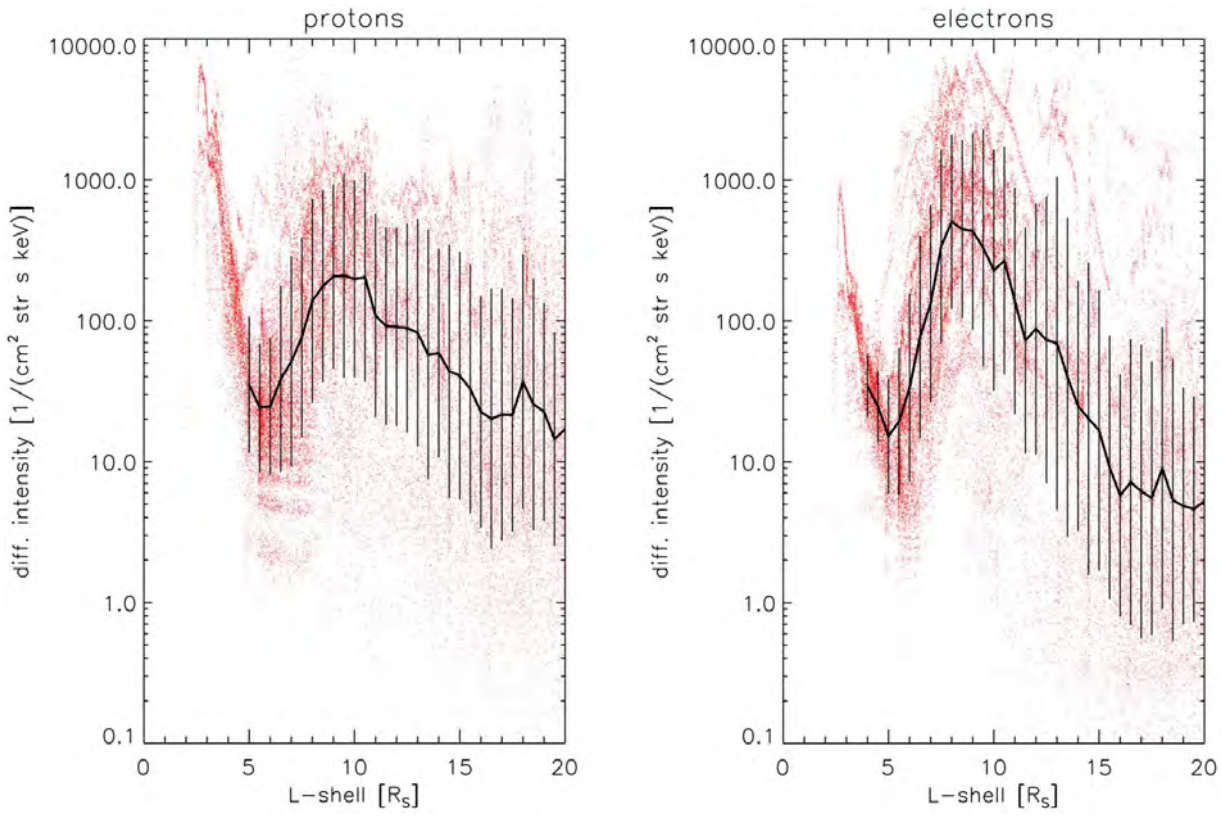

Figure 1. Differential intensities $\bar{j}$ of (left) protons and (right) electrons. Protons have mean energies of 46 keV, and electrons have mean energies of 91 keV; both species have equatorial pitch angles of α_0 = 10° ± 10°. The red points represent single measurements taken between July 2004 and June 2010 (with exceptions, see section 2). The black solid line is the logarithmic average of these points within intervals of 0.5 R_S width. Error bars show the associated 1σ standard deviations. The increase of intensities for $L < 5$ is caused by penetrating background and does not represent particles at the mentioned energies.

Figure S4. Figure 4 from Christon et al. (2014)

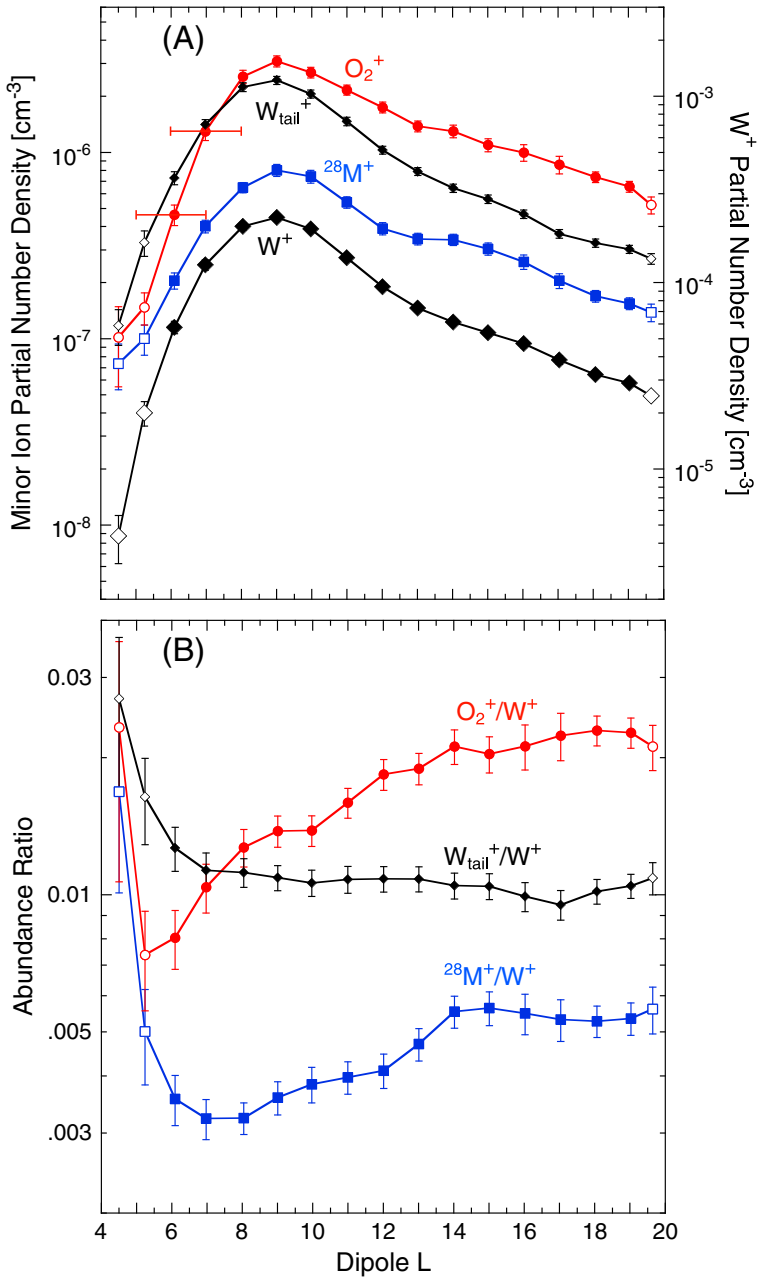

Figure 4. Running dipole *L* averages stepped every integer *L* value (with a 2 R_S window) of (a) W^+ and minor ion partial number densities, PNDs, where the right-side scale for W^+ is offset by several orders of magnitude to facilitate comparison with the minor ions and (b) abundance ratios of minor ions relative to W^+. The running averages are collected on strict integer *L* bounds and plotted at the mean distance of the average. Uncertainties shown are standard error of the means for ease of statistical comparison. Open symbols at $L < 6$ identify data currently undersampled when compared to the other *L* intervals. Open symbols at $L > 19$ identify data that may be affected by proximity to the magnetopause.

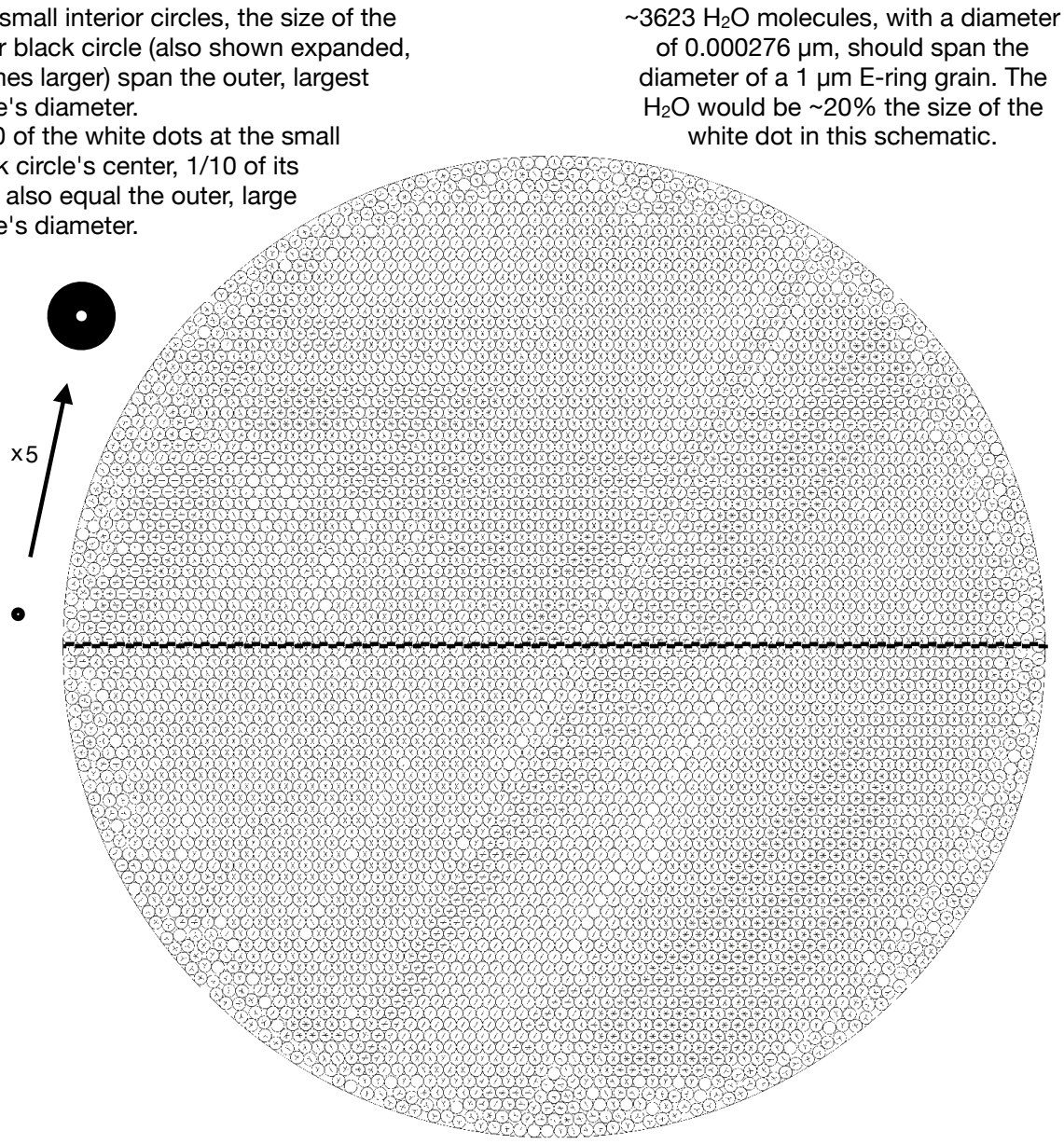

Figure S5. In order to visualize relevant ion-grain cross section scale sizes, we show an example of a large circle packed with 5000 small circles (E. Specht, 2018, The best known packings of equal circles in a circle, http://hydra.nat.uni-magdeburg.de/packing/cci/cci.html#cci5000) to represent a 1 μm E-ring grain. These interior circles are the same size as the exterior black circle that represents an enlarged version of a H_2O^+ molecule propagating into the E-ring region. An actual H_2O relative to a 1 μm E-ring grain is ~20% smaller in this comparison than the white dot size shown. Other E-ring targets are the OH molecular ions and both larger and smaller dust grains, charged both positively and negatively inside ~9 Rs (near the orbit of Rhea).