Supplementary Material

Table S1. Wavenumbers (cm^{-1}) of free OH and hydrogen bonded OH stretching modes of water as a function of the amorphous solid density (g cm^{-3}).

ρ	$\tilde{\nu}$ (free-OH)			$\tilde{\nu}$(inter)	$\tilde{\nu}$ (mixed)	$\tilde{\nu}$(intra)
0.40	3671.1	3668.2	3662.7	3341.9	3217.2	3312.5
0.50	3692.4	3688.1	3672.7	3381.4	3353.5	3270.4
0.60	3691	3686.1	3675.6	3286	3249.8	3115.9
0.75	3675.9	3670.9	3662.8	3166	3188	3008.2
1.00	3681.4	3659.6	3657.1	3122	3096.5	2917.3
1.18	3676.3	3670.4	3648.4	3138.4	3107.9	2928.2
1.60	3719.8	3655.4	3650.9	3022.2	3046.3	2798.8
1.98	3695.8	3645.5	3590.3	3175.9	3057.0	2876.8

Table. S2. Intensities (km mol^{-1}) corresponding to free OH and hydrogen bonded OH stretches of water as a function of the amorphous solid density (g cm^{-3}).

ρ	$\tilde{\nu}$ (free-OH)			$\tilde{\nu}$(inter)	$\tilde{\nu}$(mixed)	$\tilde{\nu}$(intra)
0.40	113	191	195	785	53	1006
0.50	72	151	78	150	209	2268
0.60	124	129	209	241	587	3048
0.75	94	174	228	584	544	3346
1.00	86	298	130	741	827	3400
1.18	7	227	170	1415	160	3124
1.60	137	248	193	1568	1305	3193
1.98	246	352	411	373	1830	2083

Table S3. Estimated wavenumber and intensity of the stretching modes of CH_4 and N_2 as function of the density of the sample. Activation of the forbidden v_1 mode of CH_4 is especially significant for the highest density structures. Wavenumbers in cm^{-1}, intensities in brackets in km mol^{-1}, density in g cm^{-3}.

| ρ	v_1 CH$_4$	v_3 CH$_4$	N$_2$
1.98	3041.7(27)	3190.9(4)	2041(3)
		3246.5(15)	2047(3)
		3271.2(6)	2051(1)
1.60	2985.3(78)	3114.6(32)	2030(1)
		3149.5(4)	2037(1)
		3172.9(30)	2054(5)
1.18	2931.0(18)	3048.4(23)	2038(0.3)
		3067.3(7)	2041(0.2)
		3097.1(41)	2044(0.3)
1.00	2919.1(10)	3045.5(32)	2036(2)
		3050.6(15)	2040(0)
		3056.6(6)	2042(1)
0.75	2910.7(8)	3036.5(15)	2034(0)
		3039.1(10)	2038(1)
		3049.1(6)	2041(1)
0.60	2909.9(4)	3032.4(24)	2036(0)
		3039.2(11)	2039(0)
		3047.0(9)	2039(0)
0.50	2917.5(2)	3044.7(16)	2035(0)
		3047.0(14)	2039(0)
		3048.1(17)	2039(0)
0.40	2908.4(11)	3026.1(25)	2035(0)
		3041.1(16)	2038(1)
		3047.8(10)	2039(0)
0.15	2914.6(1)	3036.4(20)	2036(0)
		3043.1(18)	2037(0)
		3052.0(4)	2038(0)
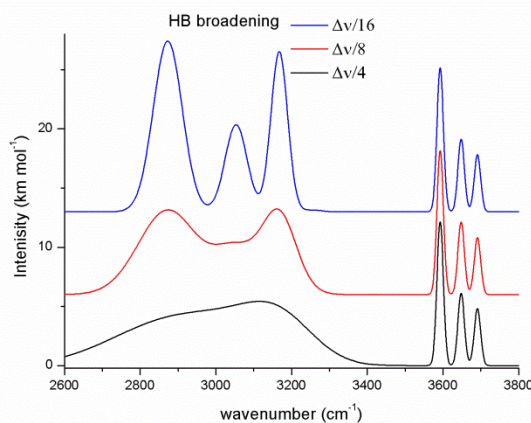
Fig. S1. Representation of the predicted spectrum of the sample with density 1.0 g cm^{-3}, using Gaussian functions of different HWHM for the HB modes, below 3400 cm^{-1}. The widths are calculated from the redshift Δv of each mode from the theoretical value of a free O-H stretching, i.e. 3600 cm^{-1}, by applying an arbitrary ratio as indicated in the figure.