Supporting data for:

Heavy Snow: IR spectroscopy of isotope mixed crystalline water ice

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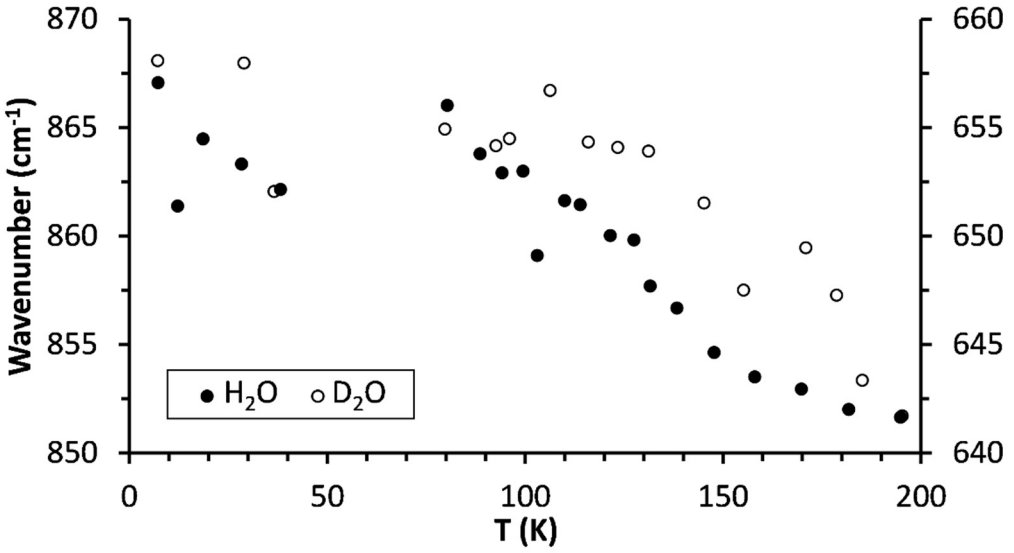
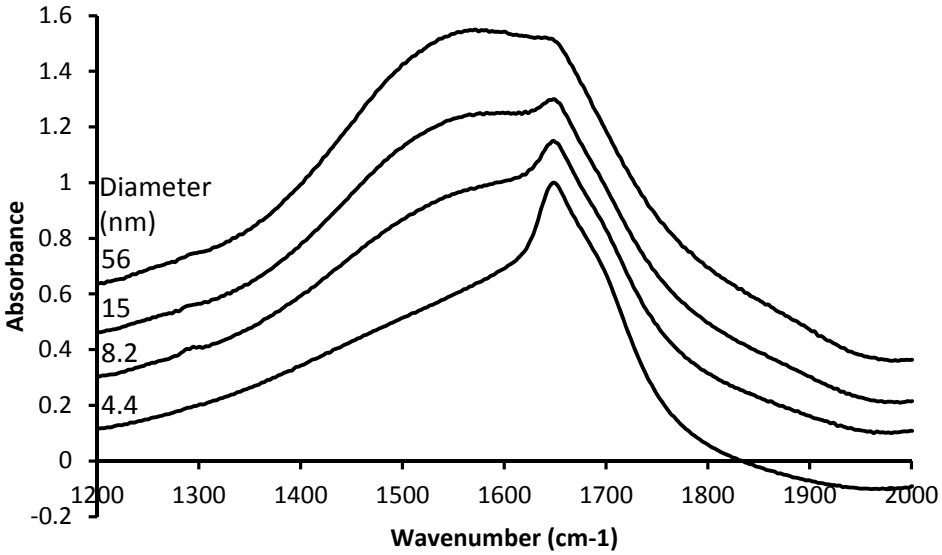
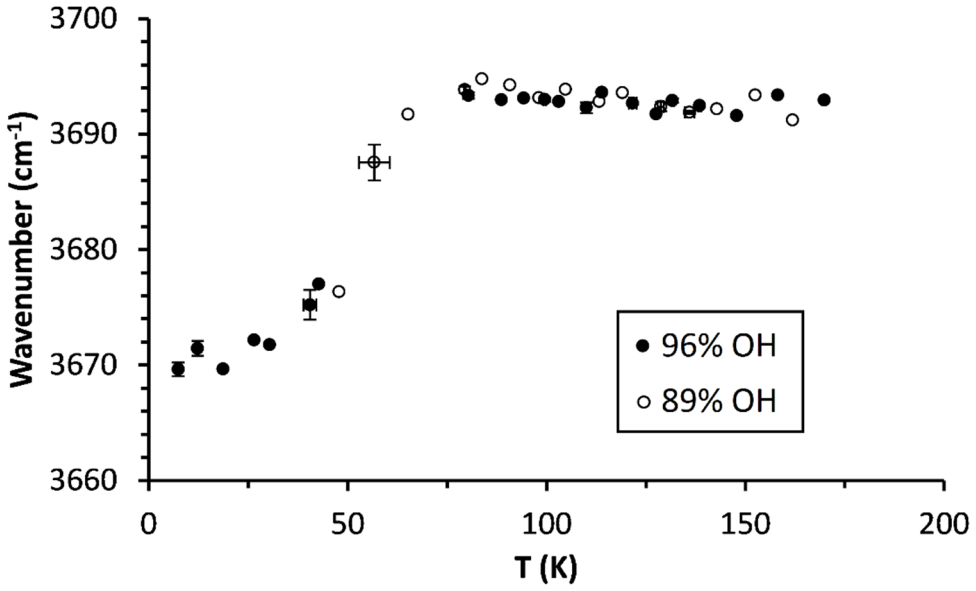


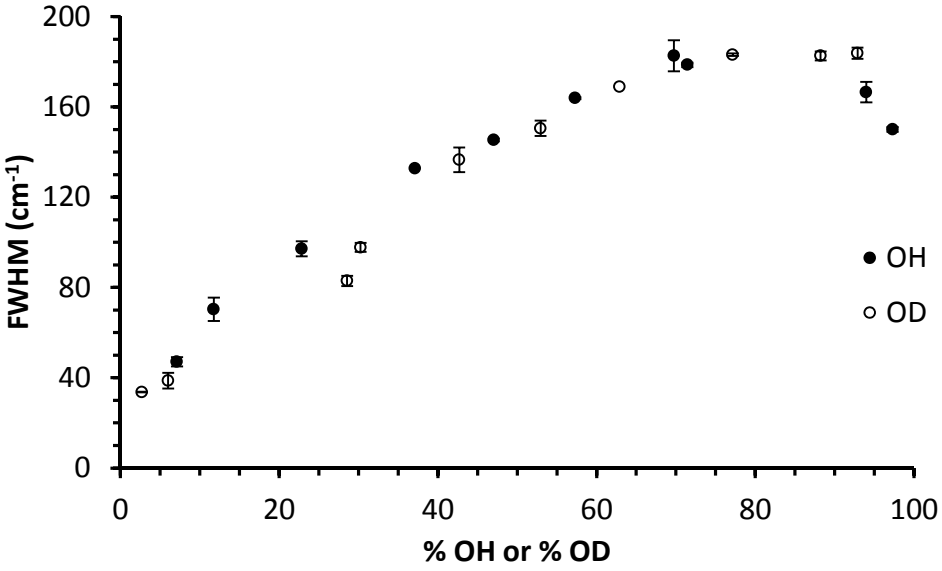
Supplementary figure S1: Comparison of the ν_L position for near pure H_2O and D_2O crystalline particles.



Supplementary figure S2: Changes in the shape of the 2 $\nu_L(H_2O)$ band as a function of increasing particle size at 78 K.



Supplementary figure S3: The COG peak position of the dOH(H_2O) band at 96±2 % OH (filled circles) and 89±3 % OH (hollow circles).



Supplementary figure S4: The FWHM of the OH and OD stretching bands as % OH (OD) is increased.

Supplementary table S1a: A more extensive list of literature values for the positions of vibrational bands for H_2O.

Reference	Phase	T (K)	ν_1 , ν_3	ν_2	ν_L	Dangling OH	Lattice TO	Lattice LA
Herzberg 1945	Vapour	--	3652/3756	1595	--	--	--	--
Giguère 1956	Cryst. Film	258	--	1650	800	--	--	--
		218	3240	1650	820	--	--	--
		103	3250	--	850	--	--	--
Hornig 1960	Cryst. Film	78	3120/3360	1585	847	--	--	--
Bayly 1963	Liquid	†	3490	1645	--	--	--	--
Whalley 1964	Cryst. Film	100	3150/3220/3380	1650	900-840	--	--	--
Ikawa 1968	Vitreous film	113	3169/3241	--	--	--	--	--
	Cryst. Film	163	3120/3206/3333	--	--	--	--	--
Bonner 1969	Liquid	†	3530	1645	--	--	--	--
Fox 1940	Liquid	†	3453	1645	--	--	--	--
Bertie 1977	Cryst. Film	78	--	--	--	--	233	230
Hasted 1977	Liquid	292	--	--	--	--	300[a]	80[a]
Rice 1978	LDA film	77	3240/3381[b]	--	--	--	--	--
	Polycryst. Film	150	3156/3219/3371[b]	--	--	--	--	--
		150	3146/3224/3359[a]	--	--	--	--	--
Devlin 1986	Cryst. Film (H_2O in D_2O)	90	3225/3270	1735	840	--	--	--
Devlin 1989	Aerosol	110	3257	--	--	--	--	--
		170	3252	--	--	--	--	--
		80	3138/3228/3348	--	--	--	--	--
Devlin 1991	Amorph. Film	15	--	--	--	3720 2cs[c]	--	--
		60	--	--	--	3696 3cs[c]	--	--
	Aerosol (in He)	80	--	--	--	3692	--	--
	Aerosol (in N_2)		--	--	--	3677	--	--

Maréchal 1991	Liquid	300	3405	1651	698	--	--	--
		348	3437	1651	682	--	--	--
Venyaminov 1997	Liquid	298	3450/3600	--	--	--	--	--
Buch 2001	Cryst. Film	12	--	--	842	--	--	--
	Aerosol (3 nm)		--	1658	842	--	--	--
	Amorph. film		--	1671	770-810	--	--	--
	Aerosol (12 nm)	100	3142/3255/3334	--	--	3676	--	--
	Aerosol (3,6,10,16,20 nm)		--	1650	--	--	--	--
	Cryst. Film		--	1560	--	--	--	--
Everest 2001	Cryst. Film	150	3225	--	830	--	--	--
Max 2002	Liquid	298	--	1638	--	--	--	--
Buch 2003	Aerosol (12 nm with CF_4)	80	--	--	868	--	--	--
	Cryst. Film	90	--	--	842	--	--	--
	Cryst. Film (H_2O in D_2O)		--	--	817/735	--	--	--
Raymond 2003	Liquid (VSF[d])	†	--	--	--	3200-3400[e]	--	--
						3703		
Ceponkus 2004	Matrix isolation (in Ne)	2.8-10	3674, 3763	1616/1599	--	--	--	--
DeRose 2004	Matrix isolation (in pH_2)	2.4	3661, 3720	1612/1622	--	--	--	--
Dlott 2004	Liquid (UNVS[f])	†	3415	1650	--	--	--	--
Millo 2005	Liquid	275	3311	1639	--	--	--	--
		271	3188	1623	--	--	--	--
Smith 2011	Amorph. Film (on Pt(111))	140	3332/3432	--	--	--	--	--
	Cryst. Film (on Pt(111))		3165/3309/3405	--	--	--	--	--
Medcraft 2012	Aerosol (in He)	5	--	--	--	--	233	166

	Aerosol (in N_2)	200	--	--	--	--	225	157
Medcraft 2013	Aerosol (in He)	78	3223	1650	*ca*. 850	3690	--	--
	Aerosol (in N_2)	209	3253	1650	860	--	--	--

† Assuming a temperature of 298 K.

[a] Determined using the imaginary component (*k*) of refractive index

[b] Determined using the imaginary component of the dielectric constant ε (=2*nk*) from thin film data.

[c] 2cs and 3cs represents 2-co-ordinated and 3-co-ordinated surface molecules respectively.

[d] VSF = vibrational sum frequency

[e] free H_2O rather than OH

[f] UNVS = ultrafast non-linear vibrational spectroscopy

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Supplementary table S1b: A more extensive list of literature values for the positions of vibrational bands for HOD.

Reference	Phase	T (K)	ν_1	ν_2	ν_3	ν_L	Dangling		Lattice	
							OH	OD	TO	LA
Hornig 1960	Cryst. Film (10% D_2O in H_2O)	78	2416	--	--	--	--	--	--	--
	Cryst. Film (50% HOD)		--	1450	--	--	--	--	--	--
	Cryst. Film (52% HOD, 49% H_2O)		2381	1477	3096/3192/3384	819	--	--	--	--
	Cryst. Film (50% HOD, 25% H_2O)		2305/2388/2463	1449	3213/3192/3370	--	--	--	--	--
	Cryst. Film (32% HOD, 4% H_2O)		2326/2408/2453	1463	3240	805	--	--	--	--
	Cryst. Film (9.5% HOD, 90.25% H_2O)		2415	--	--	--	--	--	--	--
	Cryst. Film (18% HOD, 81% H_2O)		2396/2417/2440	--	--	--	--	--	--	--
	Cryst. Film (32% HOD, 64% H_2O)		2400/2416/2444	--	--	--	--	--	--	--
Whalley 1964	Cryst. Film (HDO in H_2O)	100	2395/2421/2445	--	--	515	--	--	--	--
	Cryst. Film (HDO in D_2O)		--	--	3277	822	--	--	--	--
Ikawa 1967	Vitreous film (HOD in 90.4% D_2O)	113	2356	--	3294	--	--	--	--	--
	Cryst. Film (HOD in 3.8% D_2O)	163	2334	--	3263	--	--	--	--	--
Falk 1968	Cryst. Film (0.3% HDO in H_2O)	273	2445	--	3330	--	--	--	--	--
		78	2416	--	3260	--	--	--	--	--
	Cryst. Film (0.3% HDO in D_2O)	257	--	--	3270	--	--	--	--	--
Clarke 1971	Liquid	283	--	--	3393	--	--	--	--	--
		308	--	--	3413	--	--	--	--	--
		333	--	--	3429	--	--	--	--	--

		358	--	--	3445	--	--	--	--	--
Rice 1978	Polycryst. Film (0.5% in H_2O)	70	--	--	--	--	--	--	--	--
	Amorph. Film (0.5% in H_2O)		--	--	--	--	--	--	--	--
	Polycryst. Film (0.5% in D_2O)		--	--	3268	--	--	--	--	--
	Amorph. Film (0.5% in D_2O)		--	--	3297	--	--	--	--	--
Devlin 1986	Cryst. Film (30% $(HOD)_2$ in H_2O)	120	--	--	3238/3299	--	--	--	--	--
	Cryst. Film (30% $(HOD)_2$ in D_2O)		2396/2439	--	--	--	--	--	--	--
	Cryst. Film (30% HOD in H_2O)	90	--	1490	3270	--	--	--	--	--
	Cryst. Film (30% HOD in D_2O)		2417	1510	--	--	--	--	--	--
Devlin 1988	Polycryst. Film ($(HOD)_2$ in H_2O)	90	2442/2400	--	--	--	--	--	--	--
	Polycryst. Film (HOD in H_2O)		2420	--	--	--	--	--	--	--
Marechal 1991	Liquid (50% H to 50% D)	298	2493	1457	3391	--	--	--	--	--
	Liquid (90% H to 10% D)		2499	1457	3377	--	--	--	--	--
	Liquid (10% H to 90% D)		2471	1457	3390	--	--	--	--	--
Horn 1992	(Amorph.) Film (HOD in D_2O on Pt(111))	110	--	--	3315	--	--	--	--	--
Hage 1995	Cryst. Film (12% HOD in D_2O) 0 min	150	--	--	3285	--	--	--	--	--
	Cryst. Film (12% HOD in D_2O) 49 min		--	--	3276	--	--	--	--	--
Toth 1999	Vapour	--	2724	1403	3703	--	--	--	--	--
Buch 2000	Aerosol (18% HOD in H_2O 40 nm)	100	2389/2419/2439	--	--	--	--	--	--	--
	Aerosol (18% HOD in H_2O 4, 6, 7, 8 nm)		2415 (sub-surf)	--	--	--	--	--	--	--

	Aerosol (18% HOD in H_2O 4, 6, 7, 8 nm)		2396/2450 (surf)	--	--	--	--	--	--	--
Buch 2001	Aerosol (50% H to 50%D 8 nm)	100	--	1215	--	--	--	--	--	--
	Aerosol (18% HOD in H_2O)		--	1455	--	--	--	--	--	--
Max 2002	Liquid	298	--	1469	--	--	--	--	--	--
	Liquid (29.8% D_2O and 25.6% H_2O)		--	1446	--	--	--	--	--	--
	Liquid ('pure' HOD)		2485	1439	3370	--	--	--	--	--
Buch 2003	Aerosol in He (HOD in H_2O 12 nm)	80	--	--	--	506/515	--	--	--	--
	Aerosol in He (HOD in D_2O 12 nm)		--	--	--	824/850	--	--	--	--
Raymond 2003	Liquid (VSF[a] 0.02mf HOD, 0.25mf H_2O)	†	--	--	3200	--	3100-3450	--	--	--
Derose 2004	Matrix isolation (in pH_2)	2.4	2730	1417	3710/3723	--	--	--	--	--
Dlott 2004	Liquid (UNVS[b]) HOD in D_2O laser at 3180 cm^{-1}	†	2400/2514	1429	3393/3629	--	--	--	--	--
	Liquid (UNVS[b]) HOD in D_2O laser at 3550 cm^{-1}		2518/2371	--	3457	--	--	--	--	--
	Liquid (UNVS[b]) HOD in D_2O laser at 3380 cm^{-1}		2530	--	3455	--	--	--	--	--
Schwarzer 2006	Liquid (2% HOD in D_2O)	296	--	--	3404	--	--	--	--	--
		398	--	--	3470	--	--	--	--	--
Hamm 2011	Cryst. Film (HOD in D_2O)	80	2425	--	3272	--	--	--	--	--
Hamm 2013	Amorph. Film (HOD in D_2O)	80	2447	--	3290	--	--	--	--	--

† Assuming a temperature of 298 K.

[a] VSF = vibrational sum frequency

[b] UNVS = ultrafast non-linear vibrational spectroscopy

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Supplementary table S1c: A more extensive list of literature values for the positions of vibrational bands for D_2O.

Reference	Phase	T (K)	ν_1 , ν_3	ν_2	ν_L	Dangling OD	Lattice TO	Lattice LA
Giguère 1956	Liquid	283	--	--	530	--	--	--
	Cryst. Film	258	--		590	--	--	--
		218	2400	1210	610	--	--	--
		103	2450	1210	630	--	--	--
Hornig 1960	Cryst. Film (5% HOD in 95% D_2O)	78	2326/2408/2463	1210	--	--	--	--
Whalley 1964	Cryst. Film	110	2332/2425/2545	1210	640-675	--	--	--
Ikawa 1967	Vitreous film (90.4% D_2O)	113	2354/2433/2517	--	590	--	--	--
	Cryst. Film (90.4% D_2O)	163	2319/2417/2472	--	627	--	--	--
Bonner 1969	Liquid	†	2625	1210	--	--	--	--
Bertie 1977	Cryst. Film	78	--	--	--	--	227	--
Rice 1978	LDA film	70	2367/2435/2490[a]	--	--	--	--	--
	Polycryst. Film	150	2338/2424/2481[b]	--	--	--	--	--
			2331/2423/2480[a]	--	--	--	--	--
Devlin 1986	Cryst. Film (2% D_2O in H_2O)	90	2444/2366	1225	640	--	--	--
Devlin 1988	Polycryst. Film (D_2O in H_2O)	90	2400/2421/2442	--	--	--	--	--
		38	2325/2420/2485					
Devlin 1989	Aerosol	80	2366/2441	--	--	--	--	--
		170	2438/2500	--	--	--	--	--
		80	2339/2428/2461	--	--	--	--	--
	Aerosol (with H_2O)	90	2342, 2426	--	--	--	--	--
Devlin 1991	Amorph. Film	15	--	--	--	2748 2cs[c]	--	--
			--	--	--	2727 3cs[c]	--	--
	Amorph. Film (in He)		--	--	--	2749 2cs[c]	--	--
			--	--	--	2729 3cs[c]	--	--

	Amorph. Film (in N_2)		--	--	--	2725 2cs[c]	--	--
			--	--	--	2707 3cs[c]	--	--
	Amorph. Film (post annealing)	60	--	--	--	2727 3cs[c]	--	--
Maréchal 1991	Liquid	300	2397/2468/2548	1190	--	--	--	--
		348	2405/2500/2595	1190	--	--	--	--
Bowman 1996	Supercrit (Xe)	383	2766	--	--	--	--	--
	Supercrit (CO_2)			--	--	--	--	--
Horn 1992	Cryst. Film	110	2524	1214	--	2728	--	--
	Cryst. Film with CF_2Cl_2	--	--	--	--	2708	--	--
	Cryst. Film with CCl_3F	--	--	--	--	2702	--	--
	Cryst. Film with CCl_4	--	--	--	--	2695	--	--
Paul 1998	Vapour $(D_2O)_2$)	5	2783	--	--	--	--	--
Toth 1999	Vapour	--	2672, 2788	1178	--	--	--	--
Buch 2000	Amorph. Film	80	2370/2459/2519	--	--	--	--	--
	Aerosol (16 nm)	100	2300/2430/2490	--	--	--	--	--
Devlin 2000	Nanocryst.	136	--	--	--	2725	--	--
Buch 2001	Aerosol (20 nm with CF_4)	100	2310/2395/2515	--	--	--	--	--
	Aerosol (8 nm)		--	1211	--	--	--	--
Everest 2001	Cryst. Film (D_2O on H_2O)	145	2425	--	--	--	--	--
	Cryst. Film (D_2O on H_2O doped with HCl)		2419	--	--	--	--	--
Max 2002	Liquid (54.5% D_2O)	298	2423/2484	1200	--	--	--	--
	Liquid ('pure' D_2O)		--	1214	--	--	--	--
Buch 2003	Cryst. Film	90	--	--	633/661	--	--	--
	Aerosol (12 nm)		--	--	628/663	--	--	--
	Aerosol (12 nm isolated in H_2O)		--	--	453/504/525	--	--	--
Ceponkus 2004	Matrix isolation ($(D_2O)_2$ in Ne)	2.8 to 10	2672, 2785	1182	--	--	--	--

DeRose 2004	Matrix isolation (in pH_2)	2.4	2673, 2766	1188	--	--	--	--
Dlott 2004	Liquid (UNVS[d]) HOD in D_2O laser at 3180 cm^{-1}	†	2400/2514	1350	--	--	--	--
	Liquid (UNVS[d]) HOD in D_2O laser at 3550 cm^{-1}		2900/2371	--	--	--	--	--
	Liquid (UNVS[d]) HOD in D_2O laser at 3380 cm^{-1}		2530	--	--	--	--	--
Millo 2005	Liquid	278	2375/2475	1217	--	--	--	--
	Cryst. Film	275	2417	1217	--	--	--	--
Zasetsky 2007	Liquid	†	--	--	520	--	200	--

† Assuming a temperature of 298 K.

[a] Determined using the imaginary component of the dielectric constant ε (=2nk) from thin film data.

[b] Determined using the imaginary component (k) of refractive index.

[c] 2cs and 3cs represents 2-co-ordinated and 3-co-ordinated surface molecules respectively.

[d] UNVS = ultrafast non-linear vibrational spectroscopy.

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Supplementary table S2a: Positions of overtone and combination bands involving the ν_2, ν_L, TO and LA modes at 7 K.

Species	H_2O			HOD					D_2O		
% OH	94	81	47	94	81	47	28	3	47	28	3
Vibrational mode											
TO		235[a]				230 (78K)				227 (78K)	
LA		166 [a]				162 (78K)				161 (78K)	
ν_L in H_2O	863	846				515[b]				525[b]	
ν_L in D_2O	--	--	--	--	--	822	822	828	646	654	657
ν_2 (surf)	1653	1654	1655	--	1493	1495	--	--	--	--	--
ν_2	--	--	--	--	3224	3248	--	--	--	--	--
ν_{OH}	3218	3224	3248	--	2414	--	3263	3263	--	--	--
ν_{OD}	--	--	--	2412	--	2423	2426	--	2423	2426	2421
d_{OH}	--	3673	--	--	--	--	--	--	--	--	--
d_{OD}	3668	--	--	--	--	2705	--	--	2705	2710	2710
$2\nu_2$	--	--	--	--	--	--	--	--	--	--	--
$2\nu_L$	1573	1572	1583	--	--	--	1620	1634	1214	1215	--
$3\nu_L$	2250?	--	--	--	1984	--	1499	--	--	--	--
$\nu_2+\nu_L$	--	--	--	2250?	--	--	--	--	--	--	--

[a] C. Medcraft, D. McNaughton, C. D. Thompson, D. R. T. Appadoo, S. Bauerecker and E. G. Robertson, *Phys. Chem. Chem. Phys.*, **15**, 3630 (2013)

[b] Buch 2003: M. W. Severson, J. P. Devlin and V. Buch, *J. Chem. Phys.*, **119**, 4449 (2003)

Supplementary table S2b: Positions of overtone and combination bands involving the ν_2, ν_L, TO and LA modes at 78 K.

Species	H_2O					HOD							
% OH	94-97	70-71	57	47	37	94-97	70-71	57	47	37	23	12	7
Vibrational mode													
TO			233[a]						230 (78K)				
LA			165[a]						162 (78K)				
ν_L in H_2O	861	845	--	--	--				515[b]				
ν_L in D_2O	--	--	--	--	--	--	--	817	818	818	820	822	823
ν_2 (surf)	1648	1650	1656	1649	--	--	--	--	--	--	--	--	--
ν_2	--	--	--	--	--	--	1493	1494	1496	1500	1508	1513	1517
ν_{OH}	3227	3235	3247	--	--	--	--	--	3264	3266	3269	3269	3269
ν_{OD}	--	--	--	--	--	2416	2418	2426	2431	2430	--	--	--
d_{OH}	3691	3691	3692	3693	3692	--	--	--	3683?	--	3688	--	--
d_{OD}	--	--	--	--	--	--	--	2715	2714	2727	--	--	--
$2\nu_2$	--	--	--	--	--	--	--	--	--	--	--	--	--
$2\nu_L$	1570	1571	1573	1570	1600	--	--	--	--	--	1633?	1632	1633
$3\nu_L$	2252	--	--	--	--	--	--	--	--	--	--	--	--
$\nu_2+\nu_L$	--	--	--	--	--	2252?	1963	1966	1957	1965	--	--	--
$\nu_2+2\nu_L$	--	--	--	--	--	--	--	--	--	--	--	--	--
ν_{OH}+TO	--	--	--	--	--	--	--	--	--	--	--	3473	3473

[a] C. Medcraft, D. McNaughton, C. D. Thompson, D. R. T. Appadoo, S. Bauerecker and E. G. Robertson, *Phys. Chem. Chem. Phys.*, **15**, 3630 (2013)

[b] Buch 2003: M. W. Severson, J. P. Devlin and V. Buch, *J. Chem. Phys.*, **119**, 4449 (2003)

Supplementary table S2b cont: Positions of overtone and combination bands involving the ν_2, ν_L, TO and LA modes at 78 K.

Species	D_2O						
% OH	70-71	57	47	37	23	12	7
Vibrational mode							
TO	227 (78K)						
LA	161 (78K)						
ν_L in H_2O	525[a]						
ν_L in D_2O	--	--	--	--	--	--	658
ν_2 (surf)	--	--	--	--	--	--	--
ν_2	--	--	--	--	--	--	--
ν_{OH}	--	--	--	--	--	--	--
ν_{OD}	--	--	--	--	2432	2428	2427
d_{OH}	--	--	--	--	--	--	--
d_{OD}	--	2725	2726	2726	2726	2726	2726
$2\nu_2$	--	--	--	--	--	--	--
$2\nu_L$	1225	--	1217	1213	1210	1211	1211
$3\nu_L$	--	--	--	--	1633?	1632	1633
$\nu_2+\nu_L$	--	--	--	--	--	--	--
$\nu_2+2\nu_L$	--	--	--	--	--	--	--
ν_{OH}+TO	--	--	--	--	--	--	--

[a] Buch 2003: M. W. Severson, J. P. Devlin and V. Buch, *J. Chem. Phys.*, **119**, 4449 (2003)

Supplementary table S2c: Positions of overtone and combination bands involving the ν_2, ν_L, TO and LA modes at 140 K.

Species	H_2O					HOD							
% OH	97	77	60-65	55	47	97	77	60-65	55	47	26	12-15	7
Vibrational mode													
TO			228[a]							230 (78K)			
LA			162[a]							162 (78K)			
ν_L in H_2O	854	834	811	--	--					515[b]			
ν_L in D_2O	--	--	--	--	--	822	822	822	812	813	813	814	814
ν_2 (surf)	--	1644	--	--	--	--	--	--	--	--	--	--	--
ν_2	--	--	--	--	--	--	1490	1493	1493	1498	1499	1506	--
ν_{OH}	3236	3245	3257	--	--	--	--	--	3263	3273	3278	3278	3277
ν_{OD}	--	--	--	--	--	2423	2424	2430	2430	--	--	--	--
d_{OH}	3693	3691	3692	3692	--	--	--	--	3683	3690	3689	--	--
d_{OD}	--	--	--	--	--	--	--	--	--	2711	--	--	--
$2\nu_2$	--	--	--	--	--	--	--	--	--	2930?	2900?	2868?	--
$2\nu_L$	1567	1584	1571	1571	1574	--	--	--	--	--	1634	1629	1628
$3\nu_L$	2251	--	--	--	--	--	--	--	--	--	--	--	--
$\nu_2+\nu_L$	--	--	--	--	--	--	1958	1960	1964	1953	1923	--	--
$\nu_2+2\nu_L$	--	--	--	--	--	--	--	--	--	--	--	--	--
ν_L+TO	1118?	--	--	--	--	--	--	--	--	--	--	--	--
ν_{OH}+TO	--	--	--	--	--	--	--	--	--	--	--	--	--
ν_{OH}+LA/TO	--	--	--	--	--	--	--	--	--	--	--	3448?	3466?

[a] C. Medcraft, D. McNaughton, C. D. Thompson, D. R. T. Appadoo, S. Bauerecker and E. G. Robertson, *Phys. Chem. Chem. Phys.*, **15**, 3630 (2013)

[b] Buch 2003: M. W. Severson, J. P. Devlin and V. Buch, *J. Chem. Phys.*, **119**, 4449 (2003)

Supplementary table S2c cont: Positions of overtone and combination bands involving the ν_2, ν_L, TO and LA modes at 140 K.

Species	D_2O						
% OH	77	60-65	55	47	26	12-15	7
Vibrational mode							
TO	227 (78K)						
LA	161 (78K)						
ν_L in H_2O	525[a]						
ν_L in D_2O	--	--	--	--	--	--	--
ν_2 (surf)	--	--	--	--	--	--	--
ν_2	1222?	--	--	--	--	--	--
ν_{OH}	--	--	--	--	--	--	--
ν_{OD}	--	--	--	2437	2435	2435	2433
d_{OH}	--	--	--	--	--	--	--
d_{OD}	--	--	--	2725	2725	2725	2725
$2\nu_2$	--	--	--	--	--	--	--
$2\nu_L$	1222	1220	1220	1220	1211	1210	1211
$3\nu_L$	--	--	--	--	--	1629	--
$\nu_2+\nu_L$	--	--	--	--	--	--	--
$\nu_2+2\nu_L$	--	--	--	--	--	--	--
ν_L+TO	--	--	--	--	--	--	--
ν_{OH}+TO	--	--	--	--	--	--	--
ν_{OH}+LA/TO	--	--	--	--	--	--	--

[a] Buch 2003: M. W. Severson, J. P. Devlin and V. Buch, *J. Chem. Phys.*, **119**, 4449 (2003)

Supplementary table S2d: Positions of overtone and combination bands involving the ν_2, ν_L, TO and LA modes at 190 K.

Species	H_2O		HOD			D_2O
% OH	98	88	98	88	5	5
Vibrational mode						
TO	233[a]		--	--	--	--
LA	166[a]		--	--	--	--
ν_L in H_2O	845	836	--	--	--	--
ν_L in D_2O	--	--	--	--	804	644
ν_2 (surf)	--	--	--	--	--	--
ν_2	--	--	--	1486	1506	--
ν_{OH}	3240	3245	--	--	3288	--
ν_{OD}	--	--	2428	2429	--	2441
d_{OH}	--	--	--	--	--	--
d_{OD}	--	--	--	--	--	--
$2\nu_2$	--	--	--	--	--	--
$2\nu_L$	1561	1565	--	--	--	1207
$3\nu_L$	2247	--	--	--	--	1631
$\nu_2+\nu_L$	--	--	--	1955	--	--
$\nu_2+2\nu_L$	--	--	--	--	--	--
ν_{OH}+TO	1100?	--	--	--	--	--

[a] C. Medcraft, D. McNaughton, C. D. Thompson, D. R. T. Appadoo, S. Bauerecker and E. G. Robertson, *Phys. Chem. Chem. Phys.*, **15**, 3630 (2013)