

S2 Calculated OH stretching wavenumbers (cm⁻¹), intensities (km mol⁻¹) and assignments of the water clusters (H₂O)_n with n = 1–5 and cyclic hexmers.^a Anharmonic wavenumber calculated by the B3LYP/6-311++G(d,p) method is given in parentheses

ν	Int ^b	ν	Int ^b	ν	Int ^b	ν	Int ^b	ν	Int ^b	Assignment ^c	M_{OH}^c
Monomer		Dimer		Trimer 1		Trimer 2					
3721 (3736)	57	3716 (3730)	86	3706	99	3716	87			free ν_a	
3644 (3643)	9	3644 (3641)	16	3635	9	3643	13			free ν_s	
		3700 (3696)	80	3704	7	3716	68			free	
				3702	172	3646	14			free	
				3604	137					00DA01	-1
				3597	246					00DA01	-1
						3628	544			10DA00	-1
						3571	94			10DA00	-1
		3564 (3541)	332							00DA00	0
c-Trimer		c-Tetramer		c-Pentamer		c-Hexamer Chair		c-Hexamer Boat			
3701 (3707)	49	3695 (3692)	2	3698 (3719)	78	3696 (3700)	10	3702	69	free	
3701 (3705)	97	3694 (3692)	90	3697 (3709)	49	3696 (3701)	93	3701	75	free	
3697 (3715)	90	3694 (3693)	89	3696 (3699)	57	3695 (3700)	103	3699	57	free	
		3694 (3690)	98	3694 (3691)	76	3695 (3698)	22	3698	58	free	
				3693 (3711)	73	3695 (3718)	86	3694	93	free	
						3694 (3717)	86	3694	47	free	
3507 (3458)	528	3416 (3326)	18	3391 (3292)	40	3387 (3283)	159	3399	170	01DA10	2
3499 (3447)	573	3388 (3294)	1465	3384 (3284)	76	3374 (3267)	1	3391	36	01DA10	2
3455 (3401)	18	3387 (3294)	1466	3349 (3275)	2139	3373 (3274)	3	3375	240	01DA10	2
		3315 (3299)	0	3343 (3258)	2204	3327 (3282)	2840	3345	2358	01DA10	2
				3277 (3123)	27	3327 (3294)	2883	3329	2878	01DA10	2
						3266 (3156)	1	3279	10	01DA10	2

^a Harmonic wavenumbers calculated by the B3LYP/6-311++G(d,p) method are scaled by the formula; $\nu_{calc} = \nu_{harm}(1.184 - 0.00006 \times \nu_{harm})$.

^b Int: Infrared intensity, km mol⁻¹.

^c See text.

S3 Calculated OH stretching wavenumbers (cm^{-1}), intensities (km mol^{-1}) and assignments of the water clusters $(\text{H}_2\text{O})_n$ with $n = 6,7^a$ except cyclic hexmers

ν	Int^b	ν	Int^b	ν	Int^b	ν	Int^b	ν	Int^b	Assignment ^c	M_{OH}^c
Hexamer Bag 1		Hexamer Bag 2		Hexamer Cage		Hexamer Prism		Hexamer Book 1			
3701	102	3704	76	3702	68	3694	54	3697	67	free	
3699	60	3702	78	3695	71	3694	118	3696	71	free	
3697	60	3695	81	3694	76	3693	46	3695	75	free	
3689	78	3689	61	3690	62			3692	68	free	
3687	47							3688	66	free	
		3618	315	3595	400	3659	121	3574	412	11DA11	0
		3608	62	3571	316	3614	324			11DA11	0
				3542	167	3604	30			11DA11	0
						3563	243			11DA11	0
3543	631							3474	299	11DA10	1
3516	125	3534	250							11DA10	1
				3479	474					11DA10	1
3501	679	3511	567	3427	601			3460	828	01DA11	1
3474	169									01DA11	1
						3497	466			11DA20	2
3303	664							3417	360	01DA10	2
		3468	364			3460	431			02DA11	2
						3401	435			02DA11	2
		3434	426			=				11DA20	2
						3401	576			11DA20	2
								3335	681	01DA10	2
3241	1821	3270	1169	3391	597			3279	2162	01DA20	3
3162	723	3194	826	3358	696			3221	217	02DA10	3
				3174	827	3130	1031			02DA20	4
Hexamer Book 2		Heptamer 1		Heptamer 2		Heptamer 3		Heptamer 4			
3701	76	3715	91	3701	73	3714	90	3701	78	free	
3701	73	3696	53	3698	88	3702	72	3699	89	free	
3698	73	3696	67	3696	65	3699	22	3699	70	free	
3691	72	3695	70	3694	74	3699	108	3698	72	free	
3684	65	3692	66	3686	67	3690	69	3691	83	free	
		3643	16			3642	17	3683	67	free	
		3547	219			3540	395			12DA00	1
		3520	1047	3516	409					11DA21	1
								3522	316	00DA21	1
3495	667	3478	311	3591	236					11DA10	1
				3537	519					12DA11	1
3474	679							3488	392	01DA11	1
3461	851			3466	284					01DA11	1
3454	397					3508	815			11DA10	1
						3470	384			11DA10	1
								3474	272	01DA11	1
										11DA10	1
3430	608	3432	689	3407	443	3446	683	3453	1020	01DA10	2
3407	318	3366	1039			3426	576	3436	1195	01DA10	2
		3391	246	3489	121	3398	902			01DA21	2
				3443	1287					12DA10	2
		3327	1461					3391	472	12DA10	2
								3378	637	12DA10	2
		3238	601	3288	1081	3358	752			01DA21	2
				3206	985					01DA20	3
										02DA10	3
						3134	901			12DA20	3
								3113	1042	02DA21	3
2987	1254									02DA20	4

^a Harmonic wavenumbers calculated by the B3LYP/6-311++G(d,p) method are scaled by the formula; $\nu_{\text{calc}} = \nu_{\text{harm}}(1.184 - 0.00006 \times \nu_{\text{harm}})$.

^b Int: Infrared intensity, km mol^{-1} .

^c See text.