Table 1S Intramolecular harmonic vibrational frequency ranges of water clusters calculated with B3LYP/6-311G(d,p) [a]

W_N	ν_2	ν_1	ν_3	ν_{max}(intensity)
6A	1655-1730	3094-3654	3681-3880	3094(826)
	1662-1727[b]	3358-3772[b]	3822-3962[b]	
	1649-1708[c]	3205-3674[c]	3714-3888[c]	
6B	1652-1723	3249-3444	3876-3877	3346(2908)
	1674-1733[b]	3462-3605[b]	3953-3955[b]	
	1643-1701[c]	3303-3459[c]	3880-3882[c]	
	1767-1795[d]	3920-3986[d]	4203-4203[d]	
6C	1647-1747	3085-3686	3696-3882	3085(925)
	1659-1754[b]	3346-3788[b]	3844-3950[b]	
	1644-1718[c]	3183-3684[c]	3736-3881[c]	
10A	1659-1752	2973-3601	3616-3881	3159(3322)
	1612[e]	3452[e]	3713[e]	
10B	1658-1751	3051-3579	3586-3879	3491(1967)
10C	1660-1761	3078-3595	3610-3879	3191(4420)
10D	1628-1749	3093-3682	3715-3876	3200(4442)
20A	1658-1761	3145-3591	3615-3870	3480(2540)
20B	1545-1768	3168-3536	3596-3876	3364(2648)
20C	1659-1776	3008-3597	3620-3876	3393(3396)
20D	1680-1741	3087-3435	3700-3849	3337(3827)

[a] Frequencies are in cm^{-1}. [b] MP2/6-311+G**, ref.[1]. [c] B3LYP/TZ2P(f)++, ref. [1]. [d] HF/aug-cc-pVDZ, ref.[2]. [e] HF/6-31G(d,p) with scaling factor of 0.8929, ref. [3].

The bending bands (ν_2) do not shift significantly compared to the water monomer but are broadened to higher frequencies by about 5-150cm^{-1} except 20B of which the bending band has wider range than the others and broadens to both lower and higher frequencies. The frequencies with maximum IR intensity for all the clusters are located in the symmetric stretching band (ν_1). Significant red shifts are found for all the clusters compared to the ν_1 of water monomer. The gaps between ν_1 and ν_3 (asymmetric stretching) bands are very small. Both ν_1 and ν_2 bands are broadened but move to lower frequencies. Table 2 also lists the frequencies computed by other authors.[1,2,3]

References:

[1] J. Kim, K.S. Kim, *J. Chem. Phys.* 1998, **109**, 5886.
[2] S.S. Xantheas, T.H. Dunning, Jr. *J. Chem. Phys.* 1993, **99**, 8774.
[3] S. Maheshwary, N. Patel, N. Sathyamurthy, A.D. Kulkarni, S.R. Gadre, *J. Phys. Chem. A* 2001, **105**, 10525.