

Calculations of the IR spectra of bend fundamentals of $(\text{H}_2\text{O})_{n=3,4,5}$
using the WHBB 2 potential and dipole moment surfaces

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Supporting Information

MULTIMODE VSCF/VCI Energies and Relative Intensities of Bend on H-bonded OH-stretches for the water trimer, tetramer and pentamer.

Table S1 Trimer

Frequency (cm^{-1})	Relative Intensity
1617	0.12
1619	0.09
1634	0.03
3448	0.01
3505	0.56
3527	1.00

Table S1 Tetramer

Frequency (cm^{-1})	Relative Intensity
1635	0.07
1641	0.04
1643	0.08
1659	0.04
1666	0.00
3353	0.03
3376	0.97
3386	1.00
3416	0.06
3434	0.11

Table S2 Pentamer

Frequency (cm ⁻¹)	Relative Intensity
1635	0.07
1641	0.04
1643	0.08
1659	0.04
1666	0.00
3353	0.03
3376	0.97
3386	1.00
3416	0.06
3434	0.11