

*Supplementary results*

The origins of these calculated values are explained in Section II.4.

Table S1. Calculated vibrational magnitudes of gas phase D<sub>2</sub>O and H<sub>2</sub>O.

**H<sub>2</sub>O**

Mode	Frequency/cm <sup>-1</sup>	v <sup>a</sup>	Range <sup>b</sup> O-H <sub>1</sub> /Å	Range <sup>b</sup> O-H <sub>2</sub> /Å	Range <sup>b</sup> H <sub>1</sub> -H <sub>2</sub> /Å
v <sub>2</sub> (bend)	1595	0	0.014	0.014	0.235
		1	0.024	0.024	0.407
v <sub>1</sub> (sym. str.)	3657	0	0.135	0.135	0.215
		1	0.234	0.233	0.372
v <sub>3</sub> (asym. str.)	3756	0	0.135	0.135	0.000
		1	0.234	0.234	0.000

**D<sub>2</sub>O**

Mode	Frequency/cm <sup>-1</sup>	v <sup>a</sup>	Range <sup>b</sup> O-H <sub>1</sub> /Å	Range <sup>b</sup> O-H <sub>2</sub> /Å	Range <sup>b</sup> H <sub>1</sub> -H <sub>2</sub> /Å
v <sub>2</sub> (bend)	1178	0	0.010	0.010	0.204
		1	0.017	0.017	0.354
v <sub>1</sub> (sym. str.)	2671	0	0.115	0.115	0.174
		1	0.199	0.199	0.301
v <sub>3</sub> (asym. str.)	2788	0	0.116	0.116	0.000
		1	0.201	0.201	0.000

a. v = vibrational quantum number (0 = ground state, 1 = excited state)

b. Range X-H = difference between X-H distances at inner and outer turning points (Å)