Supporting Information:

Role of Intermolecular Charge Fluxes in the Hydrogen-Bond-Induced Frequency Shifts of the OH Stretching Mode of Water

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Supplementary figure

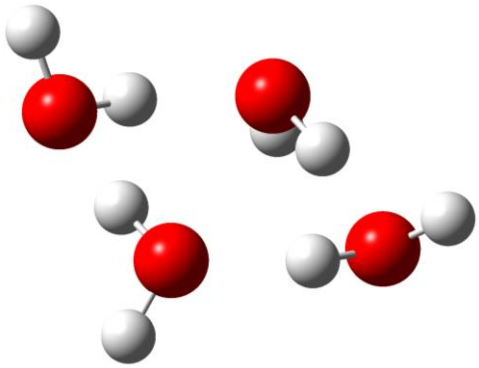

Figure S1. Structure of the water cyclic tetramer with the S_4 symmetry.

Supplementary table

Table S1. Coefficients of the polynomials of the fitting to some of the correlations among the structural, vibrational, and electrostatic properties

x	*y*	species	equation
field on H / 10^{-2} E_h e^{-1} a_0^{-1}	dipole derivative / D Å^{-1} amu$^{-1/2}$	all	$y = 0.8355\,x + 0.6313$
		non-H-bonded	$y = 0.2683\,x + 1.0753$
field on H / 10^{-2} E_h e^{-1} a_0^{-1}	frequency (scaled) / cm^{-1}	all	$y = -20.362\,x^2 - 8.534\,x + 3715.03$
hydrogen-bond distance / Å	dipole derivative / D Å^{-1} amu$^{-1/2}$	H-bonded	$y = 4.6991\,(x-2)^2 - 5.2002\,(x-2) + 2.9443$
hydrogen-bond distance / Å	frequency (scaled) / cm^{-1}	H-bonded	$y = 2612.1\,(x-2)^3 - 1563.7\,(x-2)^2 + 568.7\,(x-2) + 3520.3$