

Table 1. Experimentally Observed Isotope Effects in Water^a

property	H ₂ O	D ₂ O	T ₂ O	H ₂ ¹⁸ O	ref(s)
bond energies (kJ/mol) (gas phase)	458.9	466.4 (1.6%)			49
dipole moment (D) (gas phase)	1.855	1.855			50
vibrational frequency (cm ⁻¹) (gas phase)	3657.1	2671.6	2237.2	3649.7	51, 52
	1594.7	1178.4	995.4	1588.3	
	3755.9	2787.7	2366.6	3741.6	
water dimer dissociation energy (kJ/mol) (gas phase) 10 K	13.22	14.88 (12.7%)			53–55
melting point, <i>T</i> _m (K) (at 1 atm)	273.15	276.97 (1.40%)	277.64 (1.64%)	273.46 (0.11%)	52, 56, 57
temperature of maximum density (TMD) (K)	277.13	284.34 (2.60%)	286.55 (3.40%)	277.36 (0.08%)	58, 59
critical temperature (K)	647.10	643.85 (−0.50%)	641.66 (−0.84%)		52, 56
molar density (mol/L)	55.35	55.14 (−0.38%)	55.08 (−0.49%)	55.42 (0.13%)	56, 60
molar density at the TMD (mol/L)	55.52	55.22 (−0.53%)	55.17 (−0.63%)	55.59 (0.13%)	56, 59
liquid/vapor surface tension (N/m)	0.07198	0.07187 (−0.15%)			56
specific heat capacity, <i>C</i> _v [J/(K mol)]	74.54	84.42 (13.2%)			56, 61
translational diffusion (Å ² /ps)	0.230	0.177 (−23.0%)		0.219 (−6.1%)	62–64
rotational diffusion (rad ² /ps)	0.104	0.086 (−17%)			65
dielectric relaxation time at 20 °C (ps)	9.55	12.3 (29%)			66
viscosity (mPa s)	0.8904	1.0966 (23.2%)		0.9381 (5.4%)	56, 59
acidity pH/pD	7.00	7.43	7.6		56, 57

^aValues given are at 25 °C unless otherwise stated, and values in parentheses are percentage shifts relative to H₂O.