Water Properties (including isotopologues)

Ice Data
Spectral data

List of physicochemical data concerning water	
Property	**Data**
Area, surface covered	19.0 $Å^2$ $molecule^{-1}$ (monolayer [795]) 9.6 - 10.2 $Å^2 molecule^{-1}$(single molecule; calculated from dimensions) 8.84 $Å^2 molecule^{-1}$(single molecule; basal plane of hexagonal ice)
Atmospheric content	19.66 g kg^{-1}, 0.93 mmol L^{-1} (25 °C, 101.325 kPa, relative humidity = 100)
Bond energy, average at 0 K	H_2O, 0.5 (H-O-H ⟶ O+2H), 458.9 kJ mol bond $^{-1}$ first O-H bond dissociation energy, 492.2148 kJ mol^{-1} [350]
	D_2O, 0.5 (D-O-D ⟶ O+2D), 466.4 kJ mol bond $^{-1}$
Boiling point, 101.325 kPa	H_2O: 100.0 °C [c1] 373.1243 K (99.9743 °C), see [88]
	$H_2{}^{16}O$: 99.97 °C [745]
	$H_2{}^{17}O$: 100.08 °C [745]
	$H_2{}^{18}O$: 100.15 °C [745]
	HDO: 100.74 °C [745]
	D_2O: 101.42 °C [70]
	$D_2{}^{16}O$: 101.40 °C [745]
	$D_2{}^{18}O$: 101.54 °C [745]
	HTO: 100.8 °C [745]
	T_2O: 101.51 °C [745]
Bulk modulus (=1/κ_T, isothermal elasticity)	H_2O: 2.174 GPa (2.174 nN nm^{-2}, 25 °C); 8.9 GPa (ice 1h, -20 °C, [717])
	D_2O: 2.100 GPa (2.100 nN nm^{-2}, 25 °C)
CAS registry number	H_2O: 7732-18-5
	D_2O: 7789-20-0
	T_2O: 14940-65-9
Chemical potential (μ)	see Gibbs energy of formation
Chemical potential, temperature coefficient (dμ/dT) [987] = negative molar entropy (-S)	H_2O (gas): -188.7 J mol^{-1} K^{-1} (25 °C) H_2O (liquid): -69.9 J mol^{-1} K^{-1} (25 °C) H_2O (solid): -44.8 J mol^{-1} K^{-1} (25 °C)
Chemical potential, pressure coefficient (dμ/dP) [987] = molar volume	H_2O (gas): 24460 J mol^{-1} MPa^{-1} (25 °C) H_2O (liquid): 18.07 J mol^{-1} MPa^{-1} (25 °C) H_2O (solid): 19.73 J mol^{-1} MPa^{-1} (25 °C)
Cohesive energy density	H_2O: 2.2973 kJ cm^{-3} = 2.2973 GPa (= (ΔH_{vap}-RT)/V_M) (25 °C)
	D_2O: 2.2164 kJ cm^{-3} = 2.164 GPa (25 °C)

Internal cohesive pressure	$= \left(\frac{\partial U}{\partial V}\right)_{TPn}$ 168 MPa (25 °C), [1279] (≡ 3.04 kJ mol^{-1}, 25 °C)
Color	H_2O: very slight blue color
	D_2O: colorless
Compressibility, adiabatic (κ_S), also called isentropic compressibility	H_2O: 0.4477 GPa^{-1} (25 °C) [620], 0.5086 GPa^{-1} (0 °C) 1.158 GPa^{-1} (-20 °C), 0.2277 GPa^{-1} (250 K, 400 MPa) [2089] Ice Ih: 0.1142 GPa^{-1} (0 °C) (IAPWS)
	D_2O: 0.4625 GPa^{-1} (25 °C) [620]
Compressibility, critical ($=P_cV_c/RT_c$)	H_2O: 0.2294
	D_2O: 0.2277
Compressibility, isothermal (κ_T), $\kappa_T = -(1/V)(\delta V/\delta P)_T = <(\Delta V)^2>/(k_BTV)$ [1373b]	H_2O: 0.4599 GPa^{-1} (25 °C) [507] Ice Ih: 0.1178 GPa^{-1} (0 °C) (IAPWS); 0.069 GPa^{-1} (-20 °C), [561] gas: 10.03 MPa^{-1} (100 °C, 101.325 kPa) [540]
	D_2O: 0.4763 GPa^{-1} (25 °C) [507]
Compressibility, isothermal (κ_T), minimum	H_2O: 0.4415 GPa^{-1} at 46.5 °C, calculated from [399]
	D_2O: 0.4489 GPa^{-1} at 49.9 °C, calculated from [1454]
Compressibility, change with pressure	-0.1152 GPa^{-1} (25 °C) [1599]
Conductivity, electrolytic (IAPWS)	0.05501 µS cm^{-1} (25 °C, [737])[h], 1.2 µS cm^{-1} (22 °C, degassed; [711]) Ice Ih: ~0.06 µS cm^{-1} (-20 °C) [717] (mainly from surface defects)
Conductivity, thermal	H_2O: 0.610 W m^{-1} K^{-1} (25 °C) [IAPWS]; 0.606 502 308 W m^{-1} K^{-1} (25 °C, 0.1 MPa [IAPWS] from formula) Ice Ih: 2.4 W m^{-1} K^{-1} (-20 °C) [717] gas: 0.025 W m^{-1} K^{-1} (100 °C, 101.325 kPa) [540]
	D_2O: 0.595 W m^{-1} K^{-1} (25 °C) [IAPWS]
Conductivity, thermal; maximum	H_2O: 0.686 W m^{-1} K^{-1} at 133 °C, calculated from [1453]
	D_2O: 0.636 W m^{-1} K^{-1}at 113 °C, calculated from [1453]
Critical point (T_c, P_c, ρ_c, V_c)	H_2O: 647.096 K,[c1] 22.064 MPa, 322 kg m^{-3}, 55.9 cm^3 mol^{-1} (IAPWS)[g]
	D_2O: 643.847 K, 21.671 MPa, 356 kg m^{-3}, 56.3 cm^3 mol^{-1} (IAPWS) [g]
	T_2O: 641.657 K, 21.385 MPa, 376 kg m^{-3}, 58.6 cm^3 mol^{-1} [830] [g]
Critical point, second	H_2O: no generally accepted value, for example, ~217 K, ~340 MPa, ~1130 kg m^{-3} [419]; ~188 K, ~230 MPa, ~1100 kg m^{-3} [432]; ~182 K, ~195 MPa [580]; 145-175 K, ~200 MPa [999]; 223 K, ~50 MPa [1685]
	D_2O: ~-78 °C, ~230 MPa, ~1220 kg m^{-3} [450]; ~-86 °C,

	~211 MPa[580]		
Cryoscopic constant	H_2O: 1.8597 K kg mol^{-1}		
	$H_2^{18}O$: 2.0636 K kg mol^{-1}		
	D_2O: 2.0224 K kg mol^{-1}		
Density (25.0 °C, 101.325 kPa)	a	997.05 kg m^{-3} [67, 112], 997.047 013 kg m^{-3} (25 °C, 0.1 MPa [IAPWS] from formula)	
	H_2O	2260 kg m^{-3} (liquid, ~1500 K, 57 GPa) [1218]	
	$H_2^{17}O$	1053.12 kg m^{-3} [1006]	
	$H_2^{18}O$	1109.30 kg m^{-3} [1006]	
	HDO	1050.7 kg m^{-3} [1857]	
	D_2O	1104.36 kg m^{-3} [620]	
	$D_2^{17}O$	1159.83 kg m^{-3} [1006]	
	$D_2^{18}O$	1215.22 kg m^{-3} [1006]	
	T_2O	1213.28 kg m^{-3} [1006]	
Density of ice at melting point[a]	H_2O: 916.72 kg m^{-3} (0 °C, 101.325 kPa) (IAPWS)		
	D_2O: 1017.5 kg m^{-3} (3.82 °C)		
Density of liquid water at melting point [70]	H_2O: 999.84 kg m^{-3} (0 °C, 101.325 kPa)		
	D_2O: 1105.46 kg m^{-3} (3.813 °C)		
Density of gas at boiling point	H_2O: 0.5976 kg m^{-3} (100 °C, 101.325 kPa) [540]		
Density maximum and molecular volume at the temperature of maximum density [67,112]	a	999.97495 kg m^{-3}[e]	3.984 °C
	H_2O	999.972 kg m^{-3}, 29.91 $Å^3$ mol^{-1} 999.975 kg m^{-3} (IAPWS formula)	3.984 °C 3.978 °C (IAPWS)
	D_2O	1105.3 kg m^{-3}, 30.07 $Å^3$ mol^{-1}	11.185 °C
	T_2O	1215.01 kg m^{-3}, 30.10 $Å^3$ mol^{-1}	13.403 °C
	$H_2^{18}O$	1112.49 kg m^{-3}, 29.87 $Å^3$ mol^{-1}	4.211 °C
	$D_2^{18}O$	1216.88 kg m^{-3}, 30.06 $Å^3$ mol^{-1}	11.438 °C
Dielectric constant (more details)	H_2O: 87.9 (0 °C), 78.4 (25 °C; 78.375 218 [IAPWS] from formula at 0.1 MPa), 55.6 (100 °C) [63] 104.3 (supercooled liquid, 240 K, IAPWS) Ice Ih: 99 (-20 °C) 171 (-120 °C) [717] gas: 1.0059 (100 °C, 101.325 kPa) [540]		
	D_2O: 78.06 (25 °C) [808] D_2O Ice Ih: 104 (-20 °C) [717]		
Dielectric, change with pressure	37.88 GPa^{-1} (25 °C) [1599]		
Dielectric relaxation	H_2O: 9.55 x 10^{-12} s (20 °C) [8] H_2O Ice Ih: ~2 x 10^{-5} s (0 °C)		
	D_2O: 12.3 x 10^{-12} s (20 °C) [8]		
Diffusion coefficient	H_2O: 0.2299 $Å^2$ ps^{-1} (25 °C) [1933], 0.0187 $Å^2$ ps^{-1} (-31 °C) [62]; 6 x 10^{-8} $Å^2$ ps^{-1} (ice 1h, -20 °C) [717] ~10^{-8} $Å^2$ ps^{-1} (amorphous water, ~160 K) [334]		
	D_2O: 0.2109 $Å^2$ ps^{-1} (25 °C) [8]		

	$H_2{}^{18}O$: 0.266 $Å^2$ ps^{-1} [745]
	HDO: 0.234 $Å^2$ ps^{-1} [745]
	HTO: 0.244 $Å^2$ ps^{-1} [745]
Diffusivity, thermal $= \frac{\text{thermal conductivity}}{\text{density} \times C_p}$	H_2O: 14.6 $Å^2$ ps^{-1} (25 °C) Ice Ih: 84.3 $Å^2$ ps^{-1} (0 °C)
	D_2O: 12.7 $Å^2$ ps^{-1} (25 °C)
Dipole moment (average), μ [z]	liquid: 2.95±0.2 D (27 °C) [129] gas: 1.85498 D (6.1875×10^{-30} C m) [IAPWS], ice 1h: 3.09 D [238]
	HDO gas: 1.8517 D [IAPWS]
	D_2O gas: 1.87 D
Displacement, root mean square	~70 µm s^{-1} [1577a]
Ebullioscopic constant	H_2O: 0.5129 K kg mol^{-1}
	D_2O: 0.5626 K kg mol^{-1}
Electron affinity [563]	-16 kJ mol^{-1} (-0.17 eV) (25 °C)[l] HOMO-LUMO gap, 659 kJ mol^{-1} (6.83 eV) (25 °C)
Elemental composition, w/w [a]	H_2O: 88.8097 % oxygen, 11.1903 % hydrogen
	HDO:84.1129 % oxygen, 15.8871 % hydrogen
	D_2O:79.8866 % oxygen, 20.1134 % hydrogen
	T_2O:72.6205 % oxygen, 27.3795 % hydrogen
Energy, internal (U)	liquid: 1.8883 kJ mol^{-1} (25 °C, 101.325 kPa) [540] Ice Ih: -6.007 kJ mol^{-1} (0 °C, 101.325 kPa) (IAPWS) gas: 45.15 kJ mol^{-1} (100 °C, 101.325 kPa) [540]
Enthalpy (H = U + PV)	1.8909 kJ mol^{-1} (25 °C) [67] Ice Ih: -6.005 J mol^{-1} (0 °C, 101.325 kPa) (IAPWS) gas: 48.20 kJ mol^{-1} (100 °C, 101.325 kPa) [540]
Enthalpy of formation, ΔH_f,	H_2O liquid: -285.825 kJ mol^{-1} (25 °C) [2052]. H_2O gas: -241.831 kJ mol^{-1} (25 °C) [2052].
	D_2O: -294.6 kJmol^{-1} (25 °C) [808]
Enthalpy of vaporization (ΔH_{vap}, liquid)	H_2O: 45.051 kJ mol^{-1} (0 °C) [906], 40.657 kJ mol^{-1} (100 °C) [61] 46.567 kJmol^{-1} (240 K) [906]
	D_2O: 45.988 (3.82 °C), 41.521 kJ mol^{-1} (101.42 °C), calculated from [1453]
Enthalpy of fusion	6.00678 kJ mol^{-1} (0 °C, 101.325 kPa) [1385] 6.354 kJ mol^{-1} (81.6 °C, 2150 MPa, ice VI) [535]
	$H_2{}^{18}O$: 6.029 kJ mol^{-1} (0.31 °C) [1710]
	D_2O: 6.132 kJ mol^{-1} (3.68 °C) [2000] $D_2{}^{16}O$: 6.315 kJ mol^{-1} (3.82 °C) [1710]
	$HD^{16}O$: 6.227 kJ mol^{-1} (2.04 °C) [1710]
Enthalpy of sublimation (ice Ih)	51.059 kJmol^{-1} (0 °C), 51.139 kJ mol^{-1} (240 K) [906]
Entropy (S)	63.45 J mol^{-1} K^{-1} (Absolute entropy at triple point) [869] liquid: 6.6177 J mol^{-1} K^{-1} (25 °C) [67] Ice Ih: -21.99 J mol^{-1} K^{-1} (0 °C) (IAPWS)

	Ice Ih: 3.408 J mol^{-1} K^{-1} (0 K) [1832] ~ RLn(3/2) gas: 132.5 Jmol^{-1} K^{-1} (100 °C, 101.325 kPa) [540]
Entropy, molar	see Chemical potential, temperature coefficient (dμ/dT)
Entropy of fusion	H_2O: 22.00 J mol^{-1} K^{-1} (0 °C) [8]
	D_2O: 22.15 J mol^{-1} K^{-1} (3.68 °C) [2000]
Entropy of vaporization [8]	108.951 J mol^{-1} K^{-1} (100 °C)
Expansion coefficient (α), $\alpha_P = (1/V)(\delta V/\delta T)_P = <(\Delta V)(\Delta S)>P/(k_B^2 T)$ [1373b]	H_2O: 0.000000 $°C^{-1}$ (3.984 °C), 0.000253 $°C^{-1}$ (25 °C) [68] -0.002963 (-20 °C), +0.0004930 (250 K, 400 MPa) [2089] Ice Ih: 0.0001598 $°C^{-1}$ (0 °C, 101.325 kPa) (IAPWS); 0.000053 $°C^{-1}$ (-20 °C) [717]
	D_2O: 0.0001722 $°C^{-1}$ (25 °C) [620]
Fragile to strong liquid transition	~220 K [1200]
Gas constant (R_S)	= R/molar mass = 461.52309 J kg^{-1} K^{-1}
Gas constant (R^{95})	461.51805 J kg^{-1} K^{-1} (IAPWS)
Gibbs energy (G = U - TS + PV), all referenced to triple point	liquid: -82.157 J mol^{-1} (25 °C, 101.325 kPa) [540] Ice Ih: 1.826 J mol^{-1} (0 °C, 101.325 kPa) (IAPWS) gas: -1239 J mol^{-1} (100 °C, 101.325 kPa) [540]
Gibbs energy of formation, ΔG_f, = Chemical potential (μ)	H_2O (liquid): -237.18 kJ mol^{-1} (25 °C) [987] H_2O (gas): -228.59 kJ mol^{-1} (25 °C) [987] H_2O (solid): -236.59 kJ mol^{-1} (25 °C) [987]
	HDO (liquid): -241.86 kJ mol^{-1} (25 °C) [988] HDO (gas): -233.11 kJ mol^{-1} (25 °C) [988]
	D_2O (liquid): -243.44 kJ mol^{-1} (25 °C) [988] D_2O (gas): -234.54 kJ mol^{-1} (25 °C) [988]
Glass transition temperature	Low density liquid (~0.1 MPa): 136 K (subject to dispute [312]) High density liquid (~0.1 MPa): 110 K; 140 K at 0.2 GPa [2048]
Hardness (Mohs scale)	ice 1h: variable ~2 (0 °C), ~6 (-50 ~ -78.5 °C) [2097]
Heat capacity ratio ($\gamma=C_P/C_V$)	H_2O (gas): 1.3368 (100 °C, 101.325 kPa) [540]
Helmholtz energy (A = U - TS) [540]	liquid: -83.989 J mol^{-1} (25 °C, 101.325 kPa) Ice Ih: -0.166 J mol^{-1} (0 °C, 101.325 kPa) (IAPWS) gas: -4293 J mol^{-1} (100 °C, 101.325 kPa)
Hydrogen bond	Donor, Σα 1.17 [666]; compare $CHCl_3$, 0.15; CH_3OH, 0.43 Acceptor, Σβ; 0.47 [666]; compare $(C_2H_5)_2O$, 0.41; CH_3OH, 0.47
	Donor number (D_N), 18.0 [456]; compare CH_3CN 14.1; CH_3OH, 19.0 Acceptor number (A_N), 54.8 [456]; compare C_6H_6 8.2; CH_3OH, 41.3
Ionic dissociation constant, = $[H^+][OH^-]/[H_2O]$	H_2O: 1.821 x 10^{-16} mol l^{-1} (25 °C) [808] H_2O Ice Ih: 3.8 x 10^{-22} mol l^{-1} (-10 °C) [1831]
	D_2O: 3.54 x 10^{-17} mol l^{-1} (25 °C) [808] D_2O: Ice Ih: 1.9 x 10^{-23} mol l^{-1}(-10 °C) [1831]
	T_2O: ~1.1 x 10^{-17} mol l^{-1} (25 °C) [808]

Ionization in liquid water, ΔG (25 °C)	$2H_2O \longrightarrow H_3O^+ + OH^-$ 79.907 kJ mol^{-1} [j]
	$2D_2O \longrightarrow D_3O^+ + OD^-$ 84.88 kJ mol^{-1} [j]
Ionization potential	H_2O: gas; 1216 kJ mol^{-1} (12.61 eV) [381a] H_2O: liquid; 1018 kJ mol^{-1} (10.56 eV) [381a] H_2O: ice; 1061 kJ mol^{-1} (11.00 eV) [381a]
	D_2O: 1219 kJ mol^{-1} (12.64 eV) [381b]
Ionization rate (25 °C)	$H_2O \longrightarrow H^+ + OH^-$ $2.59x10^{-5}$ L mol^{-1} s^{-1} $H^+ + OH^- \longrightarrow H_2O$ $1.43x10^{11}$ L^2 mol^{-2} s^{-1}
Joule-Thomson coefficient (25 °C)	0.214 K MPa^{-1} [IAPWS]
Limits of stability for liquid water	Lowest temperature, -21.985 °C at 209.9 MPa Lowest pressure, 611.657 Pa at 0.01 °C Lowest density, 0.322 g cm^{-3} at 373.946 °C, 22.064 MPa Highest temperature, 373.946 °C, >22.064 MPa Highest pressure, ~12 GPa at 373.946 °C Highest density, ~1.7 g cm^{-3} at 373.946 °C, ~12 GPa
Magnetic susceptibility [670]	$-1.64x10^{-10}$ m^3 mol^{-1} (25 °C), $-1.63x10^{-10}$ m^3 mol^{-1} (0 °C)
Mass spectrum	H_2O^+ (1.0), OH^+ (0.32), H^+ (0.26), O^+ (0.07), O^{2+} (0.002), H_2^+ (0.001) (ionization cross sections at 200 eV relative to H_2O^+, [1456])
Melting, contraction on, at melting point	H_2O: 1.634 cm^3 mol^{-1}
	D_2O: 1.567 cm^3 mol^{-1}
Melting point, 101.325 kPa [70, 88]	H_2O: 0.00 °C [c2], 273.152519 K (IAPWS) 1410 K at 72 GPa [2096]
	D_2O: 3.82 °C
	T_2O: 4.49 °C
	$H_2{}^{18}O$: 273.43 K [829]
Melting point, pressure coefficient	H_2O: -74.293 mK MPa^{-1} (0 °C) [1385]
	D_2O: -68 mK MPa^{-1} (3.82 °C)
Molality [b]	H_2O: 55.508472 mol kg^{-1}
	D_2O: 49.931324 mol kg^{-1}
Molar concentration [b]	H_2O: 55.345 mol L^{-1} (25 °C)
	HOD: 55.244 mol L^{-1} (25 °C, but maximum possible is 27.3 mol L^{-1}) [1857]
	D_2O: 55.142 mol L^{-1} (25 °C)

Molar isotopic composition [a], [m]

Molar masses may be calculated	
H	1.007 825 032 07 g mol^{-1}
D	2.014 101 777 85 g mol^{-1}
T	3.016 049 2777 g mol^{-1}
^{16}O	15.994 914 619 56 g mol^{-1}
^{17}O	16.999 131 50 g mol^{-1}
^{18}O	17.999 1604 g mol^{-1}

$H_2{}^{16}O$	99.7317 % (55.21 M, 25 °C)	18.01056469 g mol^{-1}
$H_2{}^{17}O$	0.0372 % (19.51 mM, 25 °C)	19.01478156 g mol^{-1}
$H_2{}^{18}O$	0.199983 % (99.62 mM, 25 °C)	20.0148105 g mol^{-1}
$HD^{16}O$	0.031069 % (16.29 mM, 25 °C)	19.01684143 g mol^{-1}
$HD^{17}O$	0.0000116 % (5.8 µM, 25 °C)	20.02105831 g mol^{-1}

	$HD^{18}O$	0.0000623 % (29.5 μM, 25 °C)	21.0210872 g mol^{-1}
	$D_2{}^{16}O$	0.0000026 % (1.3 μM, 25 °C)	20.02311818 g mol^{-1}
	$D_2{}^{17}O$	~5 nM, 25 °C; calculated	21.02733506 g mol^{-1}
	$D_2{}^{18}O$	~26 nM, 25 °C; calculated	22.02736396 g mol^{-1}
	$HT^{16}O$	variable trace [f]	20.01878892 g mol^{-1}
	$T_2{}^{16}O$	0 % [f]	22.02701316 g mol^{-1}
Molar mass [b]	H_2O: 18.015268 g mol^{-1}		
	D_2O: 20.027508 g mol^{-1}		
Molar volume (gas, STP)	0.022199 m^3 mol^{-1} (0 °C, 101.325 kPa)		
Molecular dimensions	O-H bond length (liquid, *ab initio*), 0.991 Å [90] O-H bond length (liquid, by diffraction) 0.990 Å [1884] O-H bond length (solid ice Ih, -20 °C) , 0.985 Å [717] O-H bond length (gas, 0 K, calc.) , 0.95785 Å [836]		
	H-O-H bond angle (liquid, *ab initio*), 105.5° [90] H-O-H bond angle (solid ice Ih, -20 °C), 106.6°±1.5° [717] H-O-H bond angle (gas, 0 K, calc.), 104.50° [836]		
	O-D bond length (liquid), 0.970 Å [91], 0.985 Å [1884] O-D bond length (gas, 0 K, calc.) , 0.95783 Å [836]		
	D-O-D bond angle (liquid), 106° [91] D-O-D bond angle (gas, 0 K, calc.), 104.49° [836]		
Molecular mass	H_2O: [b] 2.9915051 x 10^{-23} g $molecule^{-1}$		
	$H_2{}^{16}O$: 2.9907243 x 10^{-23} g $molecule^{-1}$		
	$D_2{}^{16}O$: 3.3249166 x 10^{-23} g $molecule^{-1}$		
Moment of inertia (axes through centers of mass)	H_2O: 1.0220 x 10^{-40} g $cm^{2\ x}$; 2.9376 x 10^{-40} g $cm^{2\ y}$; 1.9187 x 10^{-40} g $cm^{2\ z}$ [8]		
	HDO: 1.2092 x 10^{-40} g $cm^{2\ x}$; 4.2715 x 10^{-40} g $cm^{2\ y}$; 3.0654 x 10^{-40} g $cm^{2\ z}$ [8] (z and x axes rotated around y axis by 21.09°)		
	D_2O: 1.8384 x 10^{-40} g $cm^{2\ x}$; 5.6698 x 10^{-40} g $cm^{2\ y}$; 3.8340 x 10^{-40} g $cm^{2\ z}$ [8]		
Systematic name for water	Oxidane (IUPAC); is not used. The preferred name is 'water' ^1H_2O is also known as protium oxide, when distinguishing isotopologues		
	D_2O: deuterium oxide ('heavy water')		
	T_2O: tritium oxide ('superheavy water')		
Common 'hoax' name for water	Dihydrogen monoxide (DHMO)		
NMR chemical shift, proton	H_2O liquid: 4.82 ppm H_2O ice: ~7 ppm H_2O gas: 0.56 ppm, relative to methane [850]		

	4.766 ppm for HDO in D_2O (25 °C, a triplet [609]; relative to sodium 2,2-dimethyl-2-silapentane-5-sulfonate, DSS)
NMR chemical shift, ^{17}O	H_2O liquid: 287.5 ppm (300 K, relative to O^{8+}) [886] H_2O gas: 323.6 ppm (300 K, relative to O^{8+}) [886] D $_2O$ liquid: 3.08 ppm (relative to H_2O)
Nuclear shielding constants (27 °C), [740]	^1H σ(l) 25.79 ppm (44.0 ppm parallel to O—H bond; 16.6 ppm perpendicular to O—H bond, [430]); gas to liquid shift, δ = σ(l) - σ(g) = -4.26 ppm ^{17}O σ(l) 287.5 ppm; gas to liquid shift, δ = σ(l) - σ(g) = -36.1 ppm
Octupole moment, 25 °C [452]	-1.754 D $Å^{2\ xxz}$; -0.554 D $Å^{2\ yyz}$; -1.981 D $Å^{2\ zzz}$
Octupole moment, (alternative)	linear (Ω_0) -1.34 D $Å^2$; cubic (Ω_2) 1.15 D $Å^2$; SSDQO1 [1731]$^{\Omega}$
Optical permittivity (ε_∞) [296 K, 1563]	H_2O: 2.34
	$H_2{}^{18}O$: 2.28
	D_2O: 2.29
Packing density (volume, O···O 2.82Å, 4 °C)	0.3925
pD	D_2O: 7.43 (25 °C) (based on [70])
pHD	HDO: 7.266 (25 °C)
pH	H_2O: 6.9976 (25 °C; $[H_3O]^+=[OH]^-$ = 1.0054x10^{-7} mol L^{-1}; [IAPWS])
Piezoscopic constant (= R/V_m)	H_2O: 0.4602 MPa K^{-1} (25 °C)
	D_2O: 0.4585 MPa K^{-1}(25 °C)
	T_2O: 0.4580 MPa K^{-1} (25 °C)
pK_a and pK_b	pK_a H_2O: (= pK_b H_2O) = 15.738 (25 °C) (based on [IAPWS])
	pK_a H_3O^+: (= pK_b OH^-) = -1.743 (25 °C) (calculated from H_2O molarity)
	pK_a D_2O: (= pK_b D_2O) = 16.610 (25 °C) (based on [70]))
	pK_a D_3O^+: (= pK_b OD^-) -1.741 (25 °C) (calculated from D_2O molarity)
pK_w	H_2O: 13.995 (25 °C) [IAPWS]
	D_2O: 14.87 (25 °C) [70]
Polarity/dipolarity, π [666]	1.09
Polarizability, ($\alpha = 4\pi\varepsilon_0\alpha'$)	1.62x10^{-40} F m^2
Polarizability volume , $\alpha' = \frac{\alpha}{4\pi\varepsilon_0}$	1.470 $Å^3$; 1.5284 $Å^{3\ x}$; 1.4146 $Å^{3\ y}$; 1.4679$Å^{3\ z}$ [736] 1.457 $Å^3$ (electronic), 0.037 $Å^3$ (static) [IAPWS] O-atom (1.4146 $Å^3$) H-atoms (0.0836 $Å^3$) [736]
Prandtl Number (= kinematic viscosity / thermal diffusivity)	H_2O: 6.12 (25 °C)
	D_2O: 7.81 (25 °C)
Proton spin-lattice relaxation time	T_1 = 3.6 ± 0.2 s (25 °C) [2098]
Proton spin-spin relaxation time	T_2 = 1.86 ± 0.07 s (25 °C) [2098]

Quadrupole moment, *Q*, 25 °C	-4.27 D Å [xx]; -7.99 D Å [yy]; -5.94 D Å [zz] (calc., liquid H_2O [453])
Quadrupole moment (alternative)	linear (Θ_0) 0.28 D Å; square (Θ_2) 2.13 D Å; SSDQO1 [1731][Ω]
Redox: water oxidation Redox: water reduction	$2H_2O \longrightarrow O_2(g) + 4H^+ + 4e^-$ $-E^o$ = -1.229 V (25 °C, pH 0) $2H_2O + 2e^- \longrightarrow H_2(g) + 2OH^-$ E^o = -0.8277 V (25 °C, pH 14)
Refractive index	H_2O: 1.33286 (25 °C, λ = 589.26 nm) [310] Ice Ih: η^O 1.3091; η^E 1.3105 (-3.6 °C, λ = 589 nm) [717]
	D_2O:1.32828 (20 °C, λ = 589 nm) [795]
Refractive index, real *n* and imaginary parts*k*	H_2O: *n* 1.306169; *k* 0.300352153 (25 °C, *v*, 3404.795 cm^{-1}) [942]
	D_2O: *n* 1.342528; *k* 0.279696327 (25 °C, *v*, 2503.923 cm^{-1}) [942]
Resistance, electrical	18.18 MΩ cm (25 °C, ultrapure water [737])[h], 0.8 MΩ cm (22 °C, degassed; [711])
Shear modulus (adiabatic elasticity)	H_2O: 2.44 GPa (2.44 nN nm^{-2}, 25 °C) [1326]
	D_2O: 2.50 GPa (2.50 nN nm^{-2}, 25 °C) [1326]
Specific heat capacity, $C_P = (\delta H/\delta T)_P = T(\delta S/\delta T)_P = <(\Delta S)^2>/k_B$[1373b]	H_2O: 75.338 J mol^{-1} K^{-1}; 4.1819 kJ kg^{-1} K^{-1}, 4.1696 MJ m^{-3} K^{-1} (25 °C, 101.325 kPa, calculated from [1154]), 4.181 446 18 kJ kg^{-1} K^{-1} (25 °C, 0.1 MPa [IAPWS] from formula) 108.048 J mol^{-1} K^{-1} (-20 °C), 67.687 J mol^{-1} K^{-1} (250 K, 400 MPa) [2089] Ice Ih: 37.77 J mol^{-1} K^{-1} (0 °C) (IAPWS), 22.10 J mol^{-1} K^{-1} (150 K) [906] gas: 37.47 J mol^{-1} K^{-1} (100 °C, 101.325 kPa) [540]
	D_2O: 84.67 J mol^{-1} K^{-1} ; 4.228 kJ kg^{-1} K^{-1}, 4.669 MJ m^{-3} K^{-1} (25 °C, calculated from [620])
Specific heat capacity minimum, $C_{P,min}$	H_2O: 75.27 J mol^{-1} K^{-1} at 36 °C, calculated from [1453]
	D_2O: 82.58 J mol^{-1} K^{-1} at 61 °C, calculated from [2000]
Specific heat capacity, $C_v = (\partial U/\partial T)_v$	H_2O: 74.539 J mol^{-1} K^{-1} (25 °C) [67] gas: 28.03 J mol^{-1} K^{-1} (100 °C, 101.325 kPa) [540]
	D_2O: 84.42 J mol^{-1} K^{-1} (25 °C) [620]
Speed of sound	H_2O: 1496.7 m s^{-1} (25 °C) [620], 1496.699 22 m s^{-1} (25 °C, 0.1 MPa[IAPWS] from formula); 'fast' sound ~3200 m s^{-1} [1151] 1134.6 m s^{-1} (-20 °C), 2015.9 m s^{-1} (250 K, 400 MPa) [2089] Ice Ih: 3837.9 m s^{-1} (0 °C) [1812] gas: 472.2 m s^{-1} (100 °C, 101.325 kPa) [540]
	D_2O: 1399.2 m s^{-1} (25 °C)
Speed of sound, maximum	H_2O: 1555.4 m s^{-1} at 74.0 °C, calculated from [921]
	D_2O: 1461.0 m s^{-1} at 75.6 °C, calculated from [1454]
Standard state of water	unity (exactly, as pure solvent); unit molal (as solute)
Surface entropy (= -d*γ*/dT)	H_2O: 0.1542 mJ m^{-2} K^{-1} (25 °C) (calculated from IAPWS)
Surface enthalpy (surface energy)	H_2O: 0.1179 J m^{-2} (25 °C) (= *γ* -T d*γ*/dT; calculated

	from IAPWS)
Surface tension (change with pressure) $= \left(\frac{d\gamma}{dP}\right)_{TAn} = \left(\frac{dV}{dA}\right)_{TPn}$	H_2O: 6.96 Å (25 °C) (calculated from [1279] and IAPWS)
Surface tension ($\gamma = \left(\frac{dG}{dA}\right)_{TPn}$)	H_2O (liquid - gas): 0.07198 N m^{-1}(25 °C; 0.07198 J m^{-2}) [IAPWS]
	HDO: 0.07193 N m^{-1} (25 °C; 0.07193 J m^{-2})
	D_2O: 0.07187 N m^{-1} (25 °C; 0.07187 J m^{-2}) [IAPWS]
	H_2O (ice 1h - liquid, γ_{sl}); 0.0396 N m^{-1}(0 °C; 0.0396 J m^{-2}) [2103]
	H_2O (ice 1h - gas, γ_{sg}); 0.105 N m^{-1} (0°C; 0.105 J m^{-2}) ($\gamma_{sg} \approx \gamma_{sl} + \gamma_{lg}$)
Triple point	H_2O: 0.01 °C exactly (273.16 K exactly) by definition[d] for VSMOW[a], 611.657 Pa, 0.99978 g cm^{-3} [536]
	$H_2{}^{16}O$: 0.0087 °C [565]
	$H_2{}^{17}O$: 0.21 °C [745]
	$H_2{}^{18}O$: 0.31 °C [717
	$HD^{16}O$: 2.04 °C [1710]
	D_2O: 3.80 °C, 660.096 Pa, 1.1056 g cm^{-3} [IAPWS]
	$D_2{}^{16}O$: 3.82 °C [1710]
	$D_2{}^{18}O$: 4.13 °C [745]
	HTO: 2.4 °C [745]
	T_2O: 4.49 °C [716], 662.9 Pa [830]
Van der Waals gas constants [70] [k]	a = 0.5536 Pa (m^3 $mol^{-1})^2$; b = 3.049 x 10^{-5} m^3 mol^{-1}
Vapor pressure	H_2O: 3.165 kPa (25 °C) [808]; 611.657 Pa (273.16 K, M.Pt.) [906] H_2O: 37.667 Pa (240 K) [906] Ice Ih: 611.657 Pa (273.16 K), 27.272 Pa (240 K) [906]
	D_2O: 2.734 kPa (25 °C) [808]; 659.893 Pa (276.95 K, M.Pt.) [1790]
	T_2O: 2.639 kPa (25 °C) [808]; 662.388 Pa (277.64 K, M.Pt.) [1790]
Velocity, root mean square	~640 m s^{-1} (liquid, 25 °C) [1577a]
Viscosity, dynamic	H_2O: 0.8909 mPa s (25 °C, 101.325 kPa) [IAPWS], 0.889 996 774 mPa s (25 °C, 0.1 MPa [IAPWS] from formula); gas: 0.0123 mPa s (100 °C, 101.325 kPa) [540]
	$H_2{}^{16}O$: 1.0016 mPa s (20 °C) [745]
	$H_2{}^{18}O$: 1.0564 mPa s (20 °C) [745]
	HDO: 1.1248 mPa s (20 °C) [745]
	D_2O: 1.095 mPa s (25 °C) [IAPWS]
	$D_2{}^{16}O$: 1.2467 mPa s (20 °C) [745]
	$D_2{}^{18}O$: 1.3050 mPa s (20 °C) [745]

	T_2O: 1.40 mPa s (estimated, 20 °C) [73]
Viscosity, kinematic	H_2O: 0.008935 stoke; 0.8935 x 10^{-6} m^2 s^{-1} (25 °C)
	D_2O: 0.009915 stoke; 0.9915 x 10^{-6} m^2 s^{-1} (25 °C)
Viscosity, bulk (volume viscosity)	2.47 mPa s (25 °C) [1703]
Viscosity, temperature coefficient	0.0199 mPa s K^{-1} (25 °C) [304]
Volume, molar, 101.325 kPa, V_M, see also chemical potential, pressure coefficient (dμ/dP)	H_2O liquid: 18.0182 cm^3 (0 °C) 18.0685 cm^3 (25 °C) [1006]; solid; 19.66 cm^3 (ice Ih, 0 °C); gas; 0.030143 m^3 (100 °C)
	H_2O: 50.6 $Å^3$ $molecule^{-1}$ from the van der Waals gas 'b' constant
	$H_2{}^{17}O$: 18.0556 cm^3 (25 °C) [1006]
	$H_2{}^{18}O$: 18.0428 cm^3 (25 °C) [1006]
	HDO: 18.101 cm^3 (25 °C) [1857]
	D_2O: 18.1331 cm^3 (25 °C) [1006]
	$D_2{}^{17}O$: 18.1297 cm^3 (25 °C) [1006]
	$D_2{}^{18}O$: 18.1263 cm^3 (25 °C) [1006]
	T_2O: 18.1549 cm^3 (25 °C) [1006]
Volume, intrinsic H_2O	11.01 $Å^3$
Volume, molecular H_2O at 101.325 kPa	29.92 $Å^3$ (0 °C); 32.53 $Å^3$ (ice Ih, -20 °C, [717]); 50.05 nm^3 (gas, 100 °C)
Volume, van der Waals	14.6 $Å^3$ $molecule^{-1}$ (liquid) 50.6 $Å^3$ $molecule^{-1}$ (gas, calculated from the Van der Waals gas constants)
Zero point energy	H_2O: (liquid, 25 °C) 13.9 kJ mol^{-1} [2038] H_2O: (ice 1h, 0 K) 14.6 kJ mol^{-1} [2038] H_2O: (gas, 0 K) 55.44 kJ mol^{-1} [8]
	HDO: (gas, 0 K) 48.24 kJ mol^{-1} [8]
	D_2O: (gas, 0 K) 40.54 kJ mol^{-1} [8]

[Back to Top]

Footnotes

a The Vienna Standard Mean Ocean Water (VSMOW) is pure salt-free water used as a standard material and containing 99.984426 atom % 1H, 0.015574 atom % 2H (D), 1.85 x 10-15 atom % 3H (T; equivalent to about one disintegration min-1 mol-1 water), 99.76206 atom % 16O, 0.03790 atom % 17O and 0.20004 atom % 18O [IAPWS]. Standard heavy water (D2O) has the same oxygen isotopic composition but 100% deuterium and molar mass 20.027508 g mol-1[IAPWS]. With stocks of VSMOW being used up, they have been succeeded by VSMOW2, a standardized artificial pure salt-free water isotopic mixture made to deliver the same isotopic concentrations. Two other standard water preparations exist GISP (Greenland Ice Sheet Precipitation, 0.01246 atom % 2H, 0.03313 atom % 17O, 0.1522 atom % 18O) and SLAP (Standard Light Antarctic Precipitation, 0.00905 atom % 2H, 0.02707 atom % 17O, 0.0929 atom % 18O). Standard seawater (containing salt) and its thermodynamic

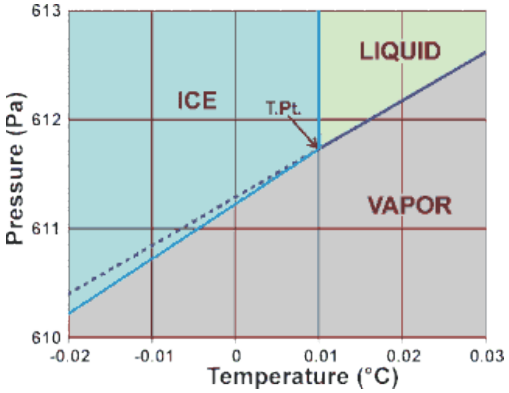
properties are described elsewhere [1452]. It should be noted that, although water contains mostly H216O, the concentrations of other isotopologues may well be greater than the solutes of interest in solutions.

The known isotopes of hydrogen and oxygen
are 1H, 2H, 3H, 4H, 5H, 6H, 7H, 12O, 13O, 14O, 15O, 16O, 17O, 18O, 19O,20O, 21O, 22O, 23O, 24O, but only 1H, 2H, 16O, 17O, 18O are stable, the rest being radioactive. Therefore, there are 9 stable isotopologues and (theoretically) 537 possible radioactive isotopologues. [Back]

b Natural isotopic mixture (VSMOW)a [IAPWS]. The density of natural water may change by up to 20 g m-3 between distillation fractions or on electrolysis; in both cases the HD18O (or D218O at higher HD18O concentrations) preferentially remaining behind. Fresh water contains less deuterium than ocean water. [Back]

c1 The boiling point of water used to be defined as 100 °C (212°F) under standard atmospheric pressure (101.325 kPa), but we now use the International Temperature Scale (ITS-90) where the boiling point is about 99.9743 °C for VSMOWa. The boiling point and critical point on the thermodynamic temperature scale have been estimated at 99.9839 °C and 647.113 K respectively [469]. [Back]

c2 The melting point of water (cold ⟶ hot) used to be defined as 0 °C (32°F) under standard atmospheric pressure (101.325 kPa), but we now use the International Temperature Scale (ITS-90). 0 °C is now defined as 273.15 K but does not exactly equal the melting point of water, 273.152519 K (IAPWS). Note that the freezing point of water (hot ⟶ cold) is ill-defined as water usually freezes a few degrees below 0 °C, the actual temperature is not reproducible. [Back]



d The precisely reproducible triple point temperature (T.Pt.) is used (employing Vienna Standard Mean Ocean Water a) to define the kelvin temperature scale (ITS-90; T.Pt. = 273.16 K exactly and the kelvin degree is 1/273.16 of the thermodynamic temperature of the triple point of VSMOW water). The Celsius scale is defined using the T.Pt. = 0.01 °C with 1 °C made identical in size to 1 K. The triple point is the temperature and pressure at which three phases (here liquid water, hexagonal ice, and water vapor) coexist at equilibrium, and will transform phase with suitable but tiny changes in temperature or pressure. Also shown, as the dashed line, is the vapor pressure of supercooled liquid water [1729]. [Back]

e The gram was once defined as exactly the mass of one cubic centimeter of water at 4 °C [Back]

f Tritium (T, 3H) has a half-life of 4500±8 days and decays by β-decay (and anti-neutrino) to 3He (${}^{3}_{1}T \rightarrow {}^{3}_{2}He^{+} + e^{-} + \overline{\nu_e}$).

Liquid T_2O undergoes self-radiolysis (~ 2.1 x 10^{15} decays s^{-1} mol^{-1} T_2O, *i.e.* ~2.1 PBq mol^{-1} T_2O). The β particles (5.7 KeV) travel only about 6 µm in water, but the antineutrinos (12.9 KeV) escape. The actual atom % of radioactive 3H in water varies between about zero, at the bottom of the oceans, to about 10-14 in atmospheric vapor; with natural abundance of about 5 x 10-15 % HTO (~2 fM, 25 °C), 6 x 10-32 % T2O [2094]. It is naturally formed by interactions between cosmic rays (for example, neutrons) and the atmosphere (for example, ${}^{14}_{7}N + n \rightarrow {}^{12}_{6}C + {}^{3}_{1}T$), falling to earth as rain (HTO). No other radioactive isotopes (for example, 15O or 14O, half lives 122 s and 71 s respectively) are found naturally in water molecules. [Back]

g The possible errors are greater than the last significant figures. [Back]

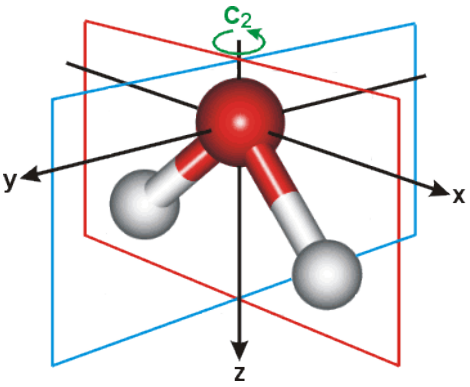
h The conductivity (that is, 1/resistance) value is made up by addition of the limiting ionic conductivities (infinite dilution) of 349.19 S cm2 mol-1and 199.24 for H+ and OH- respectively (25 °C), giving a total conductivity, which at pH=7 gives 548.43 x10-7x10-3 S cm-1 = 0.05501 µS cm-1 [737]. This corresponds to CO2-free but not degassed water [711]. The increased conductivity on degassing may be due to the removal of the non-polar gas (O2, N2) structuring effects. The conductivities of the D+ and OD- ions from D2O are about 70% and 50% of these values respectively (whether these ratios of 1/√2 and 1/2 respectively are coincidence or due to the difference in atomic mass and conductivity pathways remains to be determined). [Back]

j Calculated from $\Delta G° = -RTLn(K_w)$ where K_w is from above. This calculation assumes that the standard state of the solvent water is its mole fraction (= 1.0). Alternatively, the values may be calculated from $\Delta G° = Loge(10)xRT(pKw + 2Log10([H2O])$, where [H2O] is the molar concentration of H2O or D2O, where the standard state of the solvent water is taken as 1.0 M. This gives values of 99.78 kJ mol-1 and 104.76 kJ mol-1 for H2O and D2O respectively. [Back]

k $(P + a\left\{\frac{n}{V}\right\}^2)(V - nb) = n RT$ for n moles, with P (pressure), V (volume), R (gas constant), and T (temperature) and 'a' and 'b' are the empirical vdW constants allowing for non-ideal behavior; 'a' allowing for weak attractive interactions and 'b' arising from the finite volumes of the molecules. [Back]

l Defined as the energy to take a zero kinetic energy gas-phase electron to the bottom of the conduction band of the condensed phase as a delocalized or quasifree electron [563]. [Back]

m Molar masses vary according to source, due to isotopic fractionation during phase and chemical changes [2022]; the data does not sum to exactly 100% due to rounding errors a. [Back]



x The x direction lies in the plane of the water molecule with the origin on the oxygen and orthogonal to the H-O-H angle (that is, parallel to the longest dimension of the molecule). [Back]

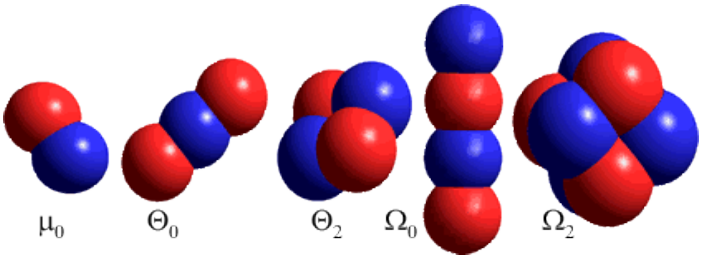
y The y direction lies orthogonal to the plane of the water molecule with the origin on the oxygen. [Back]

z The z direction lies in the plane of the water molecule with the origin on the oxygen and bisecting the H-O-H angle. [Back]

The figure right also shows the planes of symmetry (xz and yz) and the two-fold axis of rotation (C2, z-axis).

The quadrupole moments are centered on the oxygen atom (qxx= Σi cixi2 where c = charge, x = distance in x-direction and the summation is over all (i) charges). Note that calculated quadrupole moments for water vary considerably from model to model and no set of values can be considered 'correct' at the present time, except when referring to the particular model and method of calculation. Values calculated with different coordinate systems will be different (see [1731]).

The octupole moments are centered on the center of mass (oxxz= Σi cixi2zi where c = charge, x and z = distance in x- and z-directions and the summation is over all (i) charges). Note that calculated octupole moments for water vary considerably from model to model and no set of values can be considered 'correct' at the present time, except when referring to the particular model and method of calculation. Values calculated with different coordinate systems will be different (see [1731]).



Ω An alternative view of quadrupoles and octupoles [see 1731] involves the linear (Θ0) and square (Θ2) quadrupole and the linear (Ω0) and cubic (Ω2) octupole; shown in order right after the dipole (μ0) in which different charges are shown by color. [Back]

Source:http://www1.lsbu.ac.uk/water/data.html