Supporting Information

A Hydrogen-Bonding Polarizable Intermolecular Potential Model for Water

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Table S 1: Saturated density (ρ_L and ρ_v in kg/m^3), saturated vapor pressure (P in bar), enthalpy of vaporization (ΔH in kJ/mol) and vapor-liquid interfacial tension (γ in mN/m) of water calculated from the proposed HBP model. Statistical uncertainties are given in parentheses in units of the last significant figure shown: 988(2) means 988±2.

T (K)	ρ_L	ρ_v	P	ΔH	γ
298					67(3)
323	988(2)	0.067(9)	0.10(1)	45.09(3)	55(3)
373	951(1)	0.54(1)	0.88(4)	42.2(1)	
423	910(1)	2.7(1)	4.9(2)	39.2(2)	44(4)
473	859(2)	8.7(2)	16.3(4)	35.8(1)	36(3)
493	835(1)	12.4(2)	23.3(4)	34.1(1)	
513	807(2)	17.1(3)	32.9(5)	32.4(2)	
523	790(2)	20.9(4)	41.4(7)	31.4(2)	21(4)
543	761(2)	30.4(6)	58(1)	29.3(2)	
563	724(3)	42.4(7)	77(1)	26.7(2)	
573	707(2)	54(1)	92.8(8)	24.8(4)	11(3)
593	659(4)	68(2)	119(1)	21.9(4)	

Table S 2: Second virial coefficient (in L/mol) of water calculated from the proposed HBP model.

T (K)	B_2
270	-2.96
280	-2.33
290	-1.88
300	-1.54
310	-1.28
320	-1.08
330	-0.92
340	-0.799
350	-0.697
375	-0.514
400	-0.394
450	-0.254
500	-0.178

Table S 3: Energies (E in kJ/mol) and geometries, in terms of average oxygen-oxygen distance (d_{OO} in Å), of water clusters up to 6 molecules. The data for QC and BK3, GCP and TIP4P/2005 models are from reference 24. "QC" refers to the highest level quantum chemical calculations.

		QC	HBP	BK3	GCP	TIP4P/2005
Dimer	E	-20.92	-22.46	-20.63	-20.77	-28.71
	d_{OO}	2.91	2.83	2.87	2.87	2.77
Trimer	E	-66.10	-65.10	-64.23	-60.67	-76.99
	d_{OO}	2.80	2.79	2.80	2.83	2.78
Tetramer	E	-115.60	-111.20	-109.00	-106.40	-128.30
	d_{OO}		2.75	2.76	2.77	2.74
Pentamer	E	-151.80	-146.80	-143.30	-142.90	-167.30
	d_{OO}		2.74	2.74	2.74	2.74
Prism	E	-192.00	-190.10	-192.40	-181.80	-216.50
	d_{OO}		2.80	2.82	2.86	2.81
Cyclic	E	-187.40	-176.95	-175.80	-177.30	-204.20
	d_{OO}		2.76	2.74	2.74	2.74
Book	E	-190.80	-184.85	-183.00	-180.50	-212.40
	d_{OO}		2.77	2.78	2.79	2.76
Cage	E	-191.60	-186.73	-190.50	-181.90	-218.00
	d_{OO}		2.81	2.80	2.83	2.78

Table S 4: Liquid density ρ (in kg/m^3) of water at elevated pressure and temperature calculated from the HBP, BK3 and TIP4P/2005 models. Statistical uncertainties are given as in Table 1.

		ρ		
T (K)	P (bar)	HBP	BK3	TIP4P/2005
300	100	1000.5(3)	1001.1(6)	1000.5(2)
350	100	975.1(3)	978.3(3)	977.3(1)
400	100	939.3(3)	940.8(2)	939.4(2)
450	100	893.9(3)	891.4(4)	890.8(5)
500	100	835.6(2)	828.6(1)	830.6(3)
300	500	1013.0(3)	1019.3(6)	1018.6(3)
400	500	959.6(2)	960.5(1)	959.4(3)
500	500	865.2(3)	862.7(3)	863.5(2)
600	500	729.6(4)	714.6(4)	728.2(1)
700	500	464.6(8)	414(2)	515.3(8)
800	500	208.9(3)	191.6(3)	262.1(3)
300	2000	1062.4(3)	1071.4(4)	1073.3(2)
400	2000	1011.7(3)	1018.6(2)	1018.4(2)
500	2000	943.2(4)	944.9(2)	943.8(1)
600	2000	858.9(3)	855.8(2)	857.1(1)
650	2000	812.3(4)	806.4(3)	810.9(2)
700	2000	762.1(3)	754.3(3)	761.7(3)
800	2000	656.9(3)	644.8(3)	660.3(3)
900	2000	553.1(6)	541.8(2)	563.7(2)
1000	2000	467.3(4)	457.3(3)	480.3(2)

Table S 5: Isobaric heat capacity (C_p in J/mol/K) of water at 1 bar calculated from the HBP, BK3 and TIP4P/2005 models. Statistical uncertainties are given as in Table 1.

	C_p		
T (K)	HBP	BK3	TIP4P/2005
270	92(4)	97(2)	93(2)
280	88(5)	96(2)	93(2)
290		95(2)	91(2)
300	86(4)	92(3)	89(2)
310		90(3)	88(2)
320	81(4)	89(2)	86(3)
330		88(2)	87(3)
340	82(4)	86(2)	86(2)
350		85(3)	85(2)
360	78(4)	85(3)	84(2)

Table S 6: Dielectric constant (ϵ) of water at 1 bar calculated from the proposed HBP model. Statistical uncertainties are given as in Table 1.

T (K)	ϵ
270	89(5)
280	85(4)
290	83(4)
300	78(4)
310	75(3)
320	70(3)
330	66(2)
340	65(2)
350	61(2)
360	58(2)

Table S 7: Viscosity (η in cP) and self-diffusion coefficients (D in $10^{-9}\mathrm{m}^2/\mathrm{s}$) of water calculated from the HBP, BK3 and TIP4P/2005 models. Statistical uncertainties are given as in Table 1.

		HBP		BK3		TIP4P/2005	
T (K)	P (bar)	η	D	η	D	η	D
275.15	1	1.53(4)		1.91(4)		1.58(5)	
275.15	200	1.50(4)		1.83(5)		1.53(4)	
275.15	500	1.42(3)		1.78(4)		1.47(2)	
275.15	1000	1.37(2)		1.73(3)		1.41(3)	
298.15	1	0.80(4)	2.42(1)	0.95(1)	2.04(5)	0.85(2)	2.1(1)
298.15	200	0.82(3)	2.45(4)	0.96(2)	1.91(6)	0.85(2)	
298.15	480	0.829(3)	2.47(2)	0.95(2)	1.93(5)	0.84(1)	
298.15	1000	0.82(1)	2.55(4)	0.97(2)	1.9(1)	0.84(2)	
373.15	15	0.28(1)	7.74(1)	0.292(4)	7.2(1)	0.307(5)	7.5(1)
373.15	200	0.291(7)	7.32(4)	0.297(8)	7.1(1)	0.319(3)	7.4(2)
373.15	480	0.296(6)	7.52(2)	0.312(5)	6.9(2)	0.332(4)	7.4(2)
373.15	1000	0.301(2)	7.17(4)	0.32(1)	6.8(2)	0.355(7)	
523.15	200	0.110(2)	25.1(6)	0.109(3)	28(2)	0.1049(8)	25.9(9)
523.15	480	0.115(1)	25.3(3)	0.1155(8)	24.8(8)	0.130(1)	24.9(8)
523.15	1000	0.129(3)	24.2(6)	0.125(4)	22.8(7)	0.140(5)	22.7(5)