Thermodynamics of hydrogen bonding in hydrophilic and hydrophobic media

David van der Spoel[1] **Paul J. van Maaren**[1]
Per Larsson[2] **Nicuşor Tîmneanu**[1]

December 12, 2005

[1]: Dept. of Cell and Mol. Biology, Uppsala University, Husargatan 3, Box 596, SE-751 24 Uppsala, Sweden, tel: 46-18-4714205, fax: 46-18-511755, spoel@xray.bmc.uu.se

[2]: Stockholm Bioinformatics Center, Stockholm University, SE-10691 Stockholm, Sweden

Supplementary material

Table 1: Kinetics parameters k and k' (1/ps) for different MeOH concentrations and different temperatures. Numbers are averages over three different simulations, errors within parentheses.

Mass	288.15 K		298.15 K		308.15 K	
%	k	k'	k	k'	k	k'
0	0.704(0.001)	2.292(0.004)	0.832(0.001)	2.473(0.004)	0.958(0.001)	2.620(0.002)
10	0.625(0.001)	2.406(0.007)	0.749(0.001)	2.627(0.002)	0.871(0.000)	2.804(0.003)
20	0.561(0.001)	2.517(0.006)	0.680(0.001)	2.775(0.003)	0.798(0.000)	2.976(0.000)
30	0.511(0.002)	2.671(0.010)	0.621(0.001)	2.944(0.008)	0.734(0.001)	3.175(0.006)
40	0.468(0.001)	2.860(0.003)	0.572(0.001)	3.165(0.006)	0.678(0.001)	3.409(0.010)
50	0.435(0.001)	3.115(0.006)	0.532(0.001)	3.448(0.014)	0.632(0.001)	3.695(0.009)
60	0.412(0.002)	3.53(0.03)	0.501(0.001)	3.866(0.013)	0.594(0.002)	4.093(0.011)
70	0.405(0.001)	4.267(0.016)	0.482(0.004)	4.48(0.04)	0.565(0.002)	4.658(0.007)
80	0.410(0.003)	5.26(0.06)	0.479(0.002)	5.38(0.03)	0.554(0.002)	5.46(0.03)
90	0.423(0.001)	6.29(0.04)	0.486(0.001)	6.29(0.03)	0.548(0.001)	6.17(0.02)
100	0.420(0.002)	5.91(0.02)	0.487(0.001)	6.024(0.000)	0.551(0.001)	5.99(0.02)

Table 2: Kinetics parameters k and k' (1/ps) for different EtOH concentrations and different temperatures. Numbers are averages over three different simulations, errors within parentheses.

Mass	288.15 K		298.15 K		308.15 K	
%	k	k'	k	k'	k	k'
0	0.704(0.001)	2.292(0.004)	0.832(0.001)	2.473(0.004)	0.958(0.001)	2.620(0.002)
10	0.608(0.001)	2.415(0.009)	0.733(0.000)	2.646(0.004)	0.859(0.001)	2.828(0.003)
20	0.529(0.001)	2.490(0.002)	0.649(0.002)	2.765(0.007)	0.772(0.001)	2.979(0.003)
30	0.464(0.002)	2.536(0.008)	0.580(0.005)	2.86(0.03)	0.699(0.002)	3.115(0.006)
40	0.407(0.002)	2.532(0.010)	0.518(0.001)	2.901(0.006)	0.639(0.001)	3.233(0.003)
50	0.367(0.006)	2.62(0.04)	0.471(0.003)	3.009(0.016)	0.580(0.000)	3.348(0.007)
60	0.326(0.002)	2.67(0.03)	0.425(0.003)	3.13(0.03)	0.526(0.001)	3.509(0.007)
70	0.297(0.002)	2.87(0.03)	0.384(0.002)	3.330(0.013)	0.479(0.002)	3.750(0.012)
80	0.277(0.004)	3.37(0.06)	0.353(0.005)	3.83(0.05)	0.440(0.003)	4.26(0.02)
90	0.286(0.004)	4.78(0.09)	0.346(0.002)	5.03(0.04)	0.422(0.005)	5.45(0.10)
100	0.311(0.004)	6.85(0.07)	0.369(0.003)	7.08(0.06)	0.432(0.002)	7.21(0.05)

Table 3: Kinetics parameters k and k' (1/ps) for different PrOH concentrations and different temperatures. Numbers are averages over three different simulations, errors within parentheses.

Mass	288.15 K		298.15 K		308.15 K	
%	k	k'	k	k'	k	k'
0	0.704(0.001)	2.292(0.004)	0.832(0.001)	2.473(0.004)	0.958(0.001)	2.620(0.002)
10	0.617(0.001)	2.419(0.002)	0.747(0.000)	2.648(0.002)	0.874(0.000)	2.828(0.003)
20	0.558(0.004)	2.494(0.009)	0.689(0.002)	2.773(0.003)	0.811(0.001)	2.967(0.000)
30	0.515(0.004)	2.551(0.010)	0.637(0.001)	2.841(0.005)	0.757(0.001)	3.080(0.003)
40	0.477(0.003)	2.573(0.016)	0.590(0.002)	2.876(0.015)	0.712(0.003)	3.181(0.012)
50	0.432(0.002)	2.56(0.03)	0.541(0.005)	2.92(0.03)	0.659(0.004)	3.236(0.016)
60	0.380(0.002)	2.51(0.02)	0.486(0.002)	2.915(0.018)	0.602(0.003)	3.282(0.016)
70	0.333(0.003)	2.50(0.03)	0.429(0.004)	2.92(0.02)	0.543(0.002)	3.375(0.017)
80	0.283(0.003)	2.53(0.03)	0.377(0.002)	3.07(0.03)	0.478(0.005)	3.56(0.05)
90	0.255(0.006)	3.13(0.09)	0.341(0.002)	3.755(0.012)	0.428(0.005)	4.22(0.07)
100	0.330(0.004)	6.38(0.06)	0.391(0.002)	6.61(0.04)	0.461(0.002)	6.79(0.03)

Table 4: Activation thermodynamics (kJ/mol) of hydrogen bond breaking in solutions of MeOH, EtOH and PrOH as a function of concentration at T = 298.15. Errors are given within parentheses, the error in $T\Delta$S is identical to that in ΔH.

Mass	MeOH			EtOH			PrOH		
%	$\Delta G^{\ddagger}$	$\Delta H^{\ddagger}$	$T\Delta S^{\ddagger}$	$\Delta G^{\ddagger}$	$\Delta H^{\ddagger}$	$T\Delta S^{\ddagger}$	$\Delta G^{\ddagger}$	$\Delta H^{\ddagger}$	$T\Delta S^{\ddagger}$
0	4.98(0.01)	8.9(0.1)	3.9	4.98(0.01)	8.9(0.1)	3.9	4.98(0.01)	8.9(0.1)	3.9
10	5.24(0.00)	9.8(0.1)	4.5	5.30(0.00)	10.3(0.2)	5.0	5.25(0.00)	10.4(0.1)	5.2
20	5.49(0.01)	10.5(0.1)	5.0	5.60(0.01)	11.5(0.1)	5.9	5.45(0.02)	11.3(0.5)	5.8
30	5.71(0.01)	10.9(0.2)	5.2	5.88(0.06)	12.6(0.3)	6.8	5.65(0.01)	11.8(0.5)	6.1
40	5.91(0.01)	11.2(0.1)	5.3	6.16(0.02)	14.2(0.3)	8.0	5.84(0.02)	12.4(0.5)	6.5
50	6.09(0.02)	11.3(0.2)	5.2	6.40(0.05)	14.4(1.2)	8.0	6.05(0.05)	13.1(0.5)	7.1
60	6.24(0.02)	11.1(0.4)	4.8	6.65(0.05)	15.2(0.5)	8.6	6.32(0.03)	14.5(0.6)	8.2
70	6.34(0.05)	9.8(0.2)	3.4	6.90(0.04)	15.2(0.5)	8.3	6.63(0.06)	15.6(0.7)	8.9
80	6.35(0.02)	8.6(0.6)	2.3	7.11(0.09)	14.6(1.3)	7.5	6.95(0.04)	16.8(1.2)	9.9
90	6.32(0.02)	7.1(0.1)	0.7	7.16(0.04)	11.9(1.4)	4.7	7.19(0.04)	16.7(2.0)	9.5
100	6.31(0.02)	7.5(0.4)	1.2	7.00(0.05)	9.6(1.0)	2.6	6.85(0.03)	9.9(0.9)	3.0

Table 5: Equilibrium thermodynamics (kJ/mol) of hydrogen bond breaking in solutions of MeOH, EtOH and PrOH as a function of concentration at T = 298.15. Errors are given within parentheses, the error in $T\Delta$S is identical to that in ΔH.

Mass	MeOH			EtOH			PrOH		
%	ΔG	ΔH	$T\Delta$S	ΔG	ΔH	$T\Delta$S	ΔG	ΔH	$T\Delta$S
0	5.110(0.003)	9.02(0.11)	4.05	5.110(0.003)	9.02(0.11)	4.05	5.110(0.003)	9.02(0.11)	4.05
10	5.217(0.004)	9.66(0.06)	4.60	5.212(0.004)	9.87(0.06)	4.82	5.140(0.005)	9.86(0.08)	4.89
20	5.301(0.004)	10.17(0.07)	5.04	5.275(0.005)	10.49(0.08)	5.40	5.113(0.005)	10.22(0.07)	5.29
30	5.366(0.005)	10.50(0.07)	5.31	5.306(0.005)	10.94(0.09)	5.83	5.049(0.006)	10.35(0.09)	5.49
40	5.430(0.005)	10.86(0.08)	5.61	5.309(0.006)	11.40(0.11)	6.30	4.983(0.010)	10.55(0.11)	5.75
50	5.487(0.007)	11.19(0.09)	5.90	5.289(0.007)	11.58(0.12)	6.50	4.916(0.008)	10.90(0.14)	6.19
60	5.555(0.007)	11.60(0.11)	6.26	5.271(0.008)	11.72(0.14)	6.68	4.823(0.011)	10.91(0.16)	6.30
70	5.629(0.007)	11.91(0.12)	6.50	5.258(0.015)	11.93(0.15)	6.89	4.725(0.013)	11.2(0.2)	6.7
80	5.702(0.008)	12.40(0.14)	6.92	5.289(0.013)	12.30(0.19)	7.25	4.612(0.018)	11.4(0.2)	7.1
90	5.729(0.011)	12.54(0.17)	7.05	5.417(0.015)	13.2(0.3)	8.1	4.57(0.02)	12.7(0.3)	8.4
100	5.568(0.015)	12.6(0.2)	7.3	5.602(0.019)	14.4(0.3)	9.1	4.66(0.03)	14.6(0.5)	10.2