Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Cluster-Continuum Quasichemical Theory Calculation of the Lithium Ion Solvation in Water, Acetonitrile and Dimethyl Sulfoxide: Absolute Single Ion Solvation Free Energy Scales

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Table S1: Properties for solvation of anions in aqueous solution

					H2O		
HÁ	DG°(bas)	Ref.	DGsolv(HA)	Ref.	pKa(HA)	Ref.	DGsolv(A-)
HF	365.8	1	-7.57	1	3.18	1	-117.5
HCl	328.1	1	-2.2	1	-6.1	1	-87.1
HBr	318.3	1	-3.4	1	-8	1	-81.1
HI	309.2	1	-2.4	1	-9	1	-72.4
HOCl	349.2	1	-5.74	1	7.54	1	-93.1
HOBr	347.1	1	-4.58	1	8.60	1	-88.4
HOI	347.4	1	-4	1	11.64	1	-84.0
HCN	343.7	2	-3.21	1	9.22	1	-82.8
HN3	337.9	1	-3.25	1	4.70	1	-83.2
HNO2	333.7	2					
HNO3	317.8	3					
H2O	384.1	1	-6.32	1	15.74	1	-117.4
H2O2	368.6	1	-8.59	1	11.65	1	-109.8
MeOH	375.2	1	-5.10	1	15.50	1	-107.6
EtOH	371.7	1	-5.05	1	15.9	1	-103.6
i-PrOH	368.5	1	-4.80	4	17.10	4	-98.5
t-BuOH	367.7	1	-4.50	4	19.20	4	-94.5
PhOH	340.8	3	-6.62	1	9.99	1	-82.3

p-NO2-C6H4OH	320.9	3	-10.6	4	7.1	4	-70.3
HCOOH	338.3	1	-6.99	1	3.75	1	-88.7
CH3COOH	341.1	1	-6.70	1	4.76	1	-89.8
PhCOOH	333.1	1	-7.87	1	4.20	1	-83.7
CH3SO3H	315.0	1	-19.10	1	-1.2	1	-84.2
CH3NO2	349.7	1	-4.15	1	10.21	1	-88.4
CH3CHO	359.0	1	-3.50	1	16.73	1	-88.2
CH3C(=O)CH3	361.9	1	-3.85	1	19.16	1	-88.1
PhCOCH3	354.5	1	-4.58	1	18.24	1	-82.7
CH3COOEt	362.2	1	-3.10	1	25.60	1	-78.9
H2S	344.8	1	-0.44	1	7.05	1	-84.1
CH3SH	350.6	1	-1.24	1	10.33	1	-86.2
PhSH	333.8	1	-2.55	1	6.62	1	-75.8
CH3SOCH3	366.4	1	-9.8	4	33	4	-79.7
PH3	361.2	1	0.96	1	27	1	-71.9
NH3	396.9	1	-4.31	1	33	1	-104.7
PhNH2	359.1	1	-5.49	1	27	1	-76.3
HCONH2	352.8	1	-		-	1	
CH3CONH2	355.0	1	-9.71	1	15.1	1	-92.6
CH3CN	365.2	1	-3.89	1	28.9	1	-78.2
CH3CH2CN	367.9	1	-3.85	1	30.9	1	-78.1

HCCH	369.7	1	-0.01	1	21.7	1	-88.6
PhCH3	373.7	1	-		-	1	

Table S2: Properties for solvation of anions in acetonitrile solution

					ACN		
HA	ΔG^o(bas)	Ref.	ΔG_{solv}(HA)	Ref.	pK_a(HA)	Ref.	ΔG_{solv}(A-)
HF	365.8	1					
HCl	328.1	1					
HBr	318.3	1					
HI	309.2	1					
HOCl	349.2	1					
HOBr	347.1	1					
HOI	347.4	1					
HCN	343.7	2					
HN3	337.9	1					
HNO2	333.7	2					
HNO3	317.8	3	-5.7	2	8.9	2	-60.1

H2O	384.1	1					
H2O2	368.6	1					
MeOH	375.2	1					
EtOH	371.7	1					
i-PrOH	368.5	1					
t-BuOH	367.7	1					
PhOH	340.8	3	-7.5	2	27.2	6	-59.9
p-NO2-C6H4OH	320.9	3	-11.6	7	20.7	6	-53.0
HCOOH	338.3	1					
CH3COOH	341.1	1	-6.5	2	23.51	5	-64.2
PhCOOH	333.1	1	-9.4	2	21.51	5	-61.9
CH3SO3H	315.0	1					

Table S3: Properties for solvation of anions in DMSO solution

HA	ΔG^o(bas)	Ref.	ΔG_{solv}(HA)	Ref.	pK_a(HA)	Ref.	ΔG_{solv}(A-)
HF	365.8	1	-5.89	1	15	1	-92.0
HCl	328.1	1					
HBr	318.3	1					
HI	309.2	1					

HOCl	349.2	1					
HOBr	347.1	1					
HOI	347.4	1					
HCN	343.7	2	-3.15	1	12.9	1	-70.0
HN3	337.9	1	-7.05	1	7.9	1	-75.0
HNO2	333.7	2	-4.2	2	7.5	2	-68.5
HNO3	317.8	3					
H2O	384.1	1	-6.3	1	31.4	1	-88.4
H2O2	368.6	1					
MeOH	375.2	1	-5.08	1	29.0	1	-81.5
EtOH	371.7	1	-5.19	1	29.8	1	-77.0
i-PrOH	368.5	1	-5.12	1	30.3	1	-73.1
t-BuOH	367.7	1	-4.27	1	32.2	1	-68.8
PhOH	340.8	3	-7.56	1	18.0	1	-64.6
p-NO2-C6H4OH	320.9	3	-10.2	7	11.3	6	-56.4
HCOOH	338.3	1					
CH3COOH	341.1	1	-6.99	1	12.3	1	-72.1
PhCOOH	333.1	1	-10.30	2	11.0	2	-69.2
CH3SO3H	315.0	1	-11.76	1	1.6	1	-65.4
CH3NO2	349.7	1	-4.24	1	17.2	1	-71.3
CH3CHO	359.0	1					

CH3C(=O)CH3	361.9	1	-3.76	1	26.5	1	-70.3
PhCOCH3	354.5	1					
CH3COOEt	362.2	1					
H2S	344.8	1					
CH3SH	350.6	1					
PhSH	333.8	1	-3.73	1	10.3	1	-64.3
CH3SOCH3	366.4	1	-7.68	1	35.1	1	-67.0
PH3	361.2	1					
NH3	396.9	1	-1.96	1	41	1	-83.7
PhNH2	359.1	1	-6.50	1	30.6	1	-64.7
HCONH2	352.8	1	-6.73	1	23.5	1	-68.3
CH3CONH2	355.0	1	-7.63	1	25.5	1	-68.6
CH3CN	365.2	1	-3.30	1	31.3	1	-66.6
CH3CH2CN	367.9	1					
HCCH	369.7	1					
PhCH3	373.7	1	-4.42	1	43	1	-60.3

Table S4: Properties for solvation of cations in aqueous solution

					H2O		
BH+	DG°(bas)	Ref.	DGsolv(B)	Ref.	pKa(BH+)	Ref.	DGsolv(BH+)
H3O+	157.7	1	-6.32	1	-1.74	1	-97.8
CH3OH2+	173.2	1	-5.10	1	-2.05	1	-80.6
CH3CH2OH2+	178.0	1	-5.05	1	-1.94	1	-75.9
(CH3)2OH+	182.7	1	-1.90	1	-2.48	1	-67.3
(CH3CH2)2OH+	191.0	1	-1.75	1	-2.39	1	-59.0
(CH3)2C=OH+	186.9	1	-3.85	1	-3.06	1	-64.3
(PhCOCH3)H+	198.2	1	-4.58	1	-3.87	1	-52.6
(CH3COOEt)H+	192.3	1	-3.10	1	-4.61	1	-56.0
(CH3)2SH+	191.5	1	-1.54	1	-6.99	1	-52.0
(CH3SOCH3)H+	204.0	1	-10.30	1	-1.54	1	-55.7
NH4+	195.7	1	-4.31	1	9.25	1	-72.7
CH3NH3+	206.6	1	-4.57	1	10.66	1	-64.0
(CH3)2NH2+	214.3	1	-4.28	1	10.73	1	-56.1
(CH3)3NH+	219.4	1	-3.23	1	9.80	1	-48.7
EtNH3+	210.0	1	-4.51	1	10.65	1	-60.5
(Et)2NH2+	219.7	1	-4.08	1	10.84	1	-50.7
(Et)3NH+	227.0	1	-3.04	1	10.75	1	-42.2
PrNH3+	211.3	1	-4.40	1	10.54	1	-59.0

nBuNH3+	211.9	1	-4.30	1	10.66	1	-58.5
PhNH3+	203.3	1	-5.49	1	4.87	1	-60.3
pyridineH+	214.7	1	-4.69	1	5.23	1	-48.6
(HCONH2)H+	189.1	1	-9.61	1	-1.47	1	-70.0
(CH3CONH2)H+	199.0	1	-9.71	1	-0.66	1	-61.3

Table S5: Properties for solvation of cations in acetonitrile solution

					ACN		
BH+	ΔG^o(bas)	Ref.	ΔG_{solv}(B)	Ref.	pKa(BH+)	Ref.	ΔG_{solv}(BH+)
H3O+	157.7	1					
CH3OH2+	173.2	1					
CH3CH2OH2+	178.0	1					
(CH3)2OH+	182.7	1					
(CH3CH2)2OH+	191.0	1					
(CH3)2C=OH+	186.9	1					
(PhCOCH3)H+	198.2	1					
(CH3COOEt)H+	192.3	1					
(CH3)2SH+	191.5	1					
(CH3SOCH3)H+	204.0	1					

NH4+	195.7	1	-4.50	2	16.5	2	-82.6
CH3NH3+	206.6	1	-3.42	7	18.4	8	-73.2
(CH3)2NH2+	214.3	1					
(CH3)3NH+	219.4	1					
EtNH3+	210.0	1					
(Et)2NH2+	219.7	1					
(Et)3NH+	227.0	1	-3.55	7	18.50	8	-53.1
PrNH3+	211.3	1					
nBuNH3+	211.9	1					
PhNH3+	203.3	1	-7.30	2	10.60	8	-69.8
pyridineH+	214.7	1	-6.10	2	12.30	2	-59.5
(HCONH2)H+	189.1	1					
(CH3CONH2)H+	199.0	1					

Table S6: Properties for solvation of cations in DMSO solution

					DMSO		
BH+	ΔG^o(bas)	Ref.	ΔG_{solv}(B)	Ref.	pKa(BH+)	Ref.	ΔG_{solv}(BH+)
H3O+	157.7	1					
CH3OH2+	173.2	1					

CH3CH2OH2+	178.0	1					
(CH3)2OH+	182.7	1					
(CH3CH2)2OH+	191.0	1					
(CH3)2C=OH+	186.9	1					
(PhCOCH3)H+	198.2	1					
(CH3COOEt)H+	192.3	1					
(CH3)2SH+	191.5	1					
(CH3SOCH3)H+	204.0	1					
NH4+	195.7	1	-4.3	2	10.5	1	-82.1
CH3NH3+	206.6	1	-3.6	2	11.0	2	-71.2
(CH3)2NH2+	214.3	1					
(CH3)3NH+	219.4	1					
EtNH3+	210.0	1					
(Et)2NH2+	219.7	1					
(Et)3NH+	227.0	1	-2.06	1	9.07	1	-46.6
PrNH3+	211.3	1					
nBuNH3+	211.9	1	-3.37	1	11.12	1	-65.8
PhNH3+	203.3	1	-6.50	1	3.82	1	-67.6
pyridineH+	214.7	1	-4.32	1	3.40	2	-53.5
(HCONH2)H+	189.1	1					
(CH3CONH2)H+	199.0	1					

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