

醋酸离子液体[C₂mim][OAc]水溶液的摩尔表面 Gibbs 自由能

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Molar Surface Gibbs Free Energy of the Aqueous Solution of the Ionic Liquid [C₂mim][OAc]

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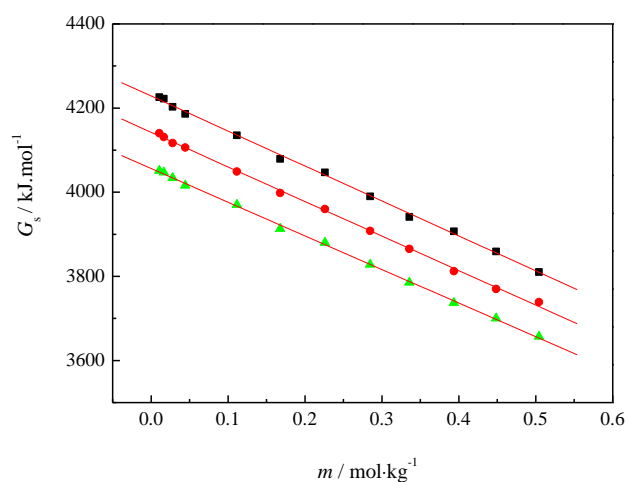


图 S1 在 288.15、298.15、308.15 和 318.15 K 温度下 G_s vs m 作图
Fig.S1 Plot of G_s vs m for aqueous $[C_2mim][OAc]$ at 293.15, 303.15 and 313.15

K

- 293.15 K: $G_s = 4229 - 831.0 m$, $r = -0.999$, $SD = 6.267$;
- 303.15 K: $G_s = 4142 - 821.6 m$, $r = -0.999$, $SD = 5.433$;
- ▲ 313.15 K: $G_s = 4056 - 799.6 m$, $r = -0.999$, $SD = 4.602$.

表S1 离子液体 $[C_2mim][OAc]$ 水溶液的平均摩尔体积

Table S1 Calculated values of average molar volume of aqueous $[C_2mim][OAc]$

$m/(\text{mol kg}^{-1})$ 1)	$10^5 V/(\text{m}^3 \text{mol}^{-1})$						
	288.15 K	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K	318.15 K
0	1.8031	1.8047	1.8068	1.8094	1.8123	1.8156	1.8193
0.0107	1.8040	1.8058	1.8080	1.8106	1.8137	1.8171	1.8209
0.0166	1.8054	1.8072	1.8094	1.8121	1.8151	1.8185	1.8223
0.0281	1.8082	1.8100	1.8122	1.8149	1.8180	1.8215	1.8253
0.0444	1.8122	1.8140	1.8163	1.8190	1.8221	1.8255	1.8293
0.1114	1.8286	1.8305	1.8329	1.8357	1.8389	1.8424	1.8462
0.1678	1.8422	1.8441	1.8466	1.8495	1.8527	1.8563	1.8602
0.2261	1.8564	1.8586	1.8610	1.8640	1.8672	1.8708	1.8748
0.2848	1.8705	1.8728	1.8753	1.8782	1.8816	1.8852	1.8892
0.3356	1.8826	1.8849	1.8876	1.8905	1.8939	1.8976	1.9017
0.3936	1.8966	1.8990	1.9016	1.9047	1.9082	1.9118	1.9159
0.4486	1.9097	1.9121	1.9148	1.9180	1.9214	1.9253	1.9293
0.5043	1.9230	1.9256	1.9283	1.9315	1.9353	1.9389	1.9430

表S2 估算的离子液体[C₂mim][OAc]水溶液的摩尔表面Gibbs自由能
Table S2 Predicted values of the molar surface Gibbs free energy for aqueous [C₂mim][OAc]

$m/(\text{mol kg}^{-1})$	$G_s(\text{est.})/(\text{J mol}^{-1})$						
	288.15	293.15	298.15	303.15	308.15	313.15	318.15
¹⁾	K	K	K	K	K	K	K
0.0107	4259	4222	4181	4136	4097	4050	4004
0.0166	4255	4217	4177	4131	4093	4046	4000
0.0281	4247	4209	4168	4123	4085	4037	3992
0.0444	4235	4197	4156	4111	4073	4026	3981
0.1114	4187	4148	4107	4063	4026	3979	3935
0.1678	4146	4107	4066	4022	3986	3939	3896
0.2261	4104	4064	4023	3980	3944	3898	3856
0.2848	4062	4021	3981	3937	3903	3857	3816
0.3356	4025	3984	3943	3900	3867	3821	3781
0.3936	3983	3942	3901	3858	3825	3780	3741
0.4486	3943	3901	3861	3818	3786	3741	3704
0.5043	3903	3861	3820	3778	3747	3702	3665

表S3 估算的离子液体[C₂mim][OAc]水溶液表面张力 $\gamma(\text{Pre})$
Table S3 The predicted values of the surface tension, $\gamma(\text{Pre})/(\text{mJ m}^{-2})$, for aqueous [C₂mim][OAc]

$m/(\text{mol} \cdot \text{kg}^{-1})$	$\gamma(\text{Pre})/(\text{mJ m}^{-2})$						
	288.15	293.15	298.15	303.15	308.15	313.15	318.15
	K	K	K	K	K	K	K
0.0107	73.3	72.6	71.8	71.0	70.2	69.3	68.5
0.0166	73.2	72.5	71.7	70.9	70.1	69.2	68.4
0.0281	72.9	72.2	71.5	70.6	69.9	69.0	68.1
0.0444	72.6	71.9	71.1	70.3	69.6	68.7	67.8
0.1114	71.2	70.5	69.8	68.9	68.2	67.3	66.5
0.1678	70.1	69.4	68.6	67.8	67.1	66.2	65.4
0.2261	68.9	68.2	67.5	66.6	66.0	65.1	64.3
0.2848	67.8	67.0	66.3	65.5	64.9	64.0	63.2
0.3356	66.8	66.0	65.3	64.5	63.9	63.1	62.3
0.3936	65.6	64.9	64.2	63.4	62.8	62.0	61.2
0.4486	64.6	63.9	63.1	62.4	61.8	61.0	60.3
0.5043	63.5	62.8	62.1	61.3	60.7	59.9	59.3

表 S4 其它离子液体水溶液的摩尔表面Gibbs自由能(g_s)Table S4 The molar surface Gibbs free energy, g_s , of aqueous solution of other aqueous ILs

$m/(\text{mol} \cdot \text{kg}^{-1})$	$g_s/(\text{J mol}^{-1})$						
	288.15 K	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K	318.15 K
Aqueous [C ₃ mim][Gly]							
0.0167	4258	4213	4168	4130	4085	4037	3995
0.0278	4255	4209	4165	4126	4082	4034	3992
0.0444	4250	4204	4159	4121	4078	4029	3988
0.0556	4247	4201	4156	4118	4075	4026	3985
0.1112	4229	4182	4138	4099	4059	4011	3969
0.1670	4211	4163	4119	4080	4043	3995	3953
0.2229	4192	4144	4100	4061	4027	3979	3937
0.2789	4173	4123	4079	4040	4009	3962	3919
0.3351	4152	4102	4059	4019	3991	3944	3901
0.3913	4132	4081	4037	3997	3972	3926	3882
0.4477	4110	4058	4015	3975	3953	3907	3863
0.5041	4088	4035	3992	3952	3933	3887	3843
Aqueous [C ₄ mim][Gly]							
0.0167	4251	4206	4171	4132	4088	4041	4000
0.0278	4248	4203	4168	4129	4085	4038	3998
0.0444	4244	4199	4163	4124	4081	4034	3994
0.0556	4242	4196	4160	4120	4078	4032	3991
0.1112	4228	4181	4143	4103	4063	4018	3978
0.1670	4213	4165	4126	4085	4048	4004	3963
0.2229	4197	4149	4107	4067	4032	3989	3948
0.2789	4181	4131	4089	4047	4015	3974	3933
0.3351	4164	4113	4069	4027	3997	3957	3916
0.3913	4146	4095	4049	4006	3979	3941	3899
0.4477	4128	4075	4027	3984	3960	3923	3881
0.5041	4109	4055	4006	3962	3940	3905	3863
Aqueous [C ₄ mim][Pro]							
0.0111	4256	4218	4175	4132	4090	4048	4001
0.0278	4241	4209	4166	4123	4075	4039	3986
0.0556	4209	4176	4139	4102	4059	4023	3970
0.1112	4178	4151	4119	4076	4021	3985	3931
0.1670	4139	4107	4075	4025	3982	3934	3904
0.2789	4054	4015	3983	3933	3896	3853	3810
0.3351	4001	3962	3929	3891	3842	3792	3749
0.3912	3935	3901	3869	3830	3780	3737	3705
0.4470	3898	3858	3819	3786	3736	3704	3673
Aqueous [C ₅ mim][Pro]							
0.0111	4251	4213	4175	4133	4085	4043	4002

0.0278	4248	4210	4167	4118	4076	4034	3987
0.0557	4205	4173	4141	4092	4056	4020	3978
0.1112	4182	4126	4123	4051	4020	3984	3930
0.1670	4134	4084	4081	4020	3971	3928	3886
0.2774	4046	4001	3993	3931	3881	3844	3801
0.3350	3995	3956	3942	3873	3835	3798	3730
0.3913	3931	3885	3883	3807	3763	3725	3682
0.4477	3889	3843	3835	3771	3720	3682	3644
Aqueous [C ₆ mim][Pro]							
0.0115	4246	4208	4170	4127	4079	4038	3996
0.0277	4238	4200	4156	4119	4071	4029	3988
0.0547	4207	4163	4119	4082	4052	4010	3962
0.1112	4151	4107	4093	4043	4013	3970	3916
0.1673	4100	4061	4047	3991	3942	3923	3881
0.2789	4015	3982	3956	3899	3844	3819	3781
0.3350	3978	3926	3906	3861	3787	3767	3724
0.3910	3920	3886	3835	3778	3740	3696	3652
0.4475	3874	3828	3764	3725	3693	3661	3623

表S5 估算的其它离子液体水溶液的摩尔表面Gibbs自由能($g_s(\text{est.})$)
Table S5 The predicted values of the molar surface Gibbs free energy, $g_s(\text{est.})$, of other aqueous ILs

$m/(\text{mol} \cdot \text{kg}^{-1})$	$g_s(\text{est.})/(\text{J mol}^{-1})$						
	288.15 K	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K	318.15 K
Aqueous [C ₃ mim][Gly]							
0.0167	4261	4215	4170	4132	4088	4039	3998
0.0278	4257	4211	4166	4128	4084	4036	3994
0.0444	4251	4205	4160	4122	4079	4030	3989
0.0556	4247	4201	4157	4118	4076	4027	3986
0.1112	4228	4181	4137	4098	4058	4010	3968
0.1670	4209	4161	4117	4078	4041	3993	3951
0.2229	4189	4141	4097	4058	4024	3976	3934
0.2789	4170	4121	4077	4037	4007	3959	3916
0.3351	4150	4100	4057	4017	3989	3942	3899
0.3913	4131	4080	4037	3997	3972	3925	3882
0.4477	4111	4059	4016	3976	3954	3908	3864
0.5041	4092	4039	3996	3956	3937	3891	3847
Aqueous [C ₄ mim][Gly]							
0.0167	4254	4208	4173	4135	4090	4043	4003
0.0278	4250	4205	4170	4131	4087	4040	4000
0.0444	4246	4200	4164	4125	4082	4035	3995
0.0556	4242	4197	4160	4121	4079	4032	3992
0.1112	4226	4180	4142	4102	4062	4017	3976

0.1670	4210	4162	4123	4083	4045	4002	3961
0.2229	4194	4145	4104	4063	4029	3986	3945
0.2789	4178	4128	4086	4044	4012	3971	3930
0.3351	4162	4111	4067	4025	3995	3955	3914
0.3913	4146	4094	4048	4005	3978	3940	3898
0.4477	4129	4077	4029	3986	3961	3924	3883
0.5041	4113	4059	4010	3966	3944	3909	3867

Aqueous [C₄mim][Pro]

0.0111	4257	4224	4186	4142	4097	4057	4006
0.0278	4243	4211	4172	4128	4084	4044	3993
0.0556	4221	4188	4150	4106	4061	4021	3972
0.1112	4176	4142	4104	4062	4016	3976	3929
0.1670	4130	4096	4059	4017	3971	3931	3886
0.2789	4040	4004	3968	3928	3881	3840	3800
0.3351	3994	3957	3923	3883	3836	3794	3757
0.3912	3948	3911	3877	3838	3790	3749	3714
0.4470	3903	3865	3832	3794	3745	3703	3671

Aqueous [C₅mim][Pro]

0.0111	4257	4216	4186	4136	4095	4055	4009
0.0278	4243	4202	4173	4122	4081	4041	3995
0.0557	4220	4179	4152	4099	4058	4018	3972
0.1112	4174	4132	4109	4053	4011	3972	3925
0.1670	4128	4085	4065	4007	3964	3925	3879
0.2774	4036	3991	3980	3916	3871	3833	3786
0.3350	3988	3943	3935	3868	3823	3785	3738
0.3913	3941	3895	3891	3822	3776	3738	3691
0.4477	3894	3848	3848	3775	3728	3691	3644

Aqueous [C₆mim][Pro]

0.0115	4243	4203	4174	4131	4088	4049	4004
0.0277	4229	4189	4160	4117	4073	4035	3989
0.0547	4207	4166	4136	4092	4049	4011	3966
0.1112	4159	4118	4086	4041	3997	3961	3916
0.1673	4111	4070	4036	3991	3946	3911	3867
0.2789	4016	3975	3938	3890	3844	3812	3769
0.3350	3969	3927	3888	3839	3793	3762	3720
0.3910	3921	3879	3839	3789	3741	3712	3671
0.4475	3873	3831	3789	3738	3690	3662	3621

表S6 预测的离子液体[C₂mim][OAc]水溶液的摩尔表面焓(*h*)

Table S6 The predicted values of the molar surface enthalpy, *h*, for aqueous [C₂mim][OAc]

<i>m</i> /(mol · kg ⁻¹)	<i>h</i> /(J mol ⁻¹)						
	288.15 K	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K	318.15 K
0.0107	1801	1721	1635	1550	1465	1375	1291
0.0166	1803	1729	1637	1552	1473	1383	1294
0.0281	1801	1721	1635	1550	1466	1382	1292
0.0444	1793	1712	1627	1548	1464	1374	1284
0.1114	1779	1699	1619	1529	1450	1366	1277
0.1678	1730	1643	1570	1479	1406	1310	1226
0.2261	1742	1662	1583	1492	1414	1330	1253
0.2848	1716	1631	1558	1467	1395	1305	1227
0.3356	1684	1598	1537	1440	1374	1278	1194
0.3936	1675	1602	1504	1426	1354	1270	1199
0.4486	1648	1569	1478	1399	1333	1250	1166
0.5043	1633	1548	1469	1397	1313	1235	1158