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288.15-318.15 K温度范围内离子液体[C_5mim][Pro]水溶液的体积和表面性质

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Volume and Surface Properties of Aqueous [C_5mim][Pro] at 288.15 to 318.15 K

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Section A ^{1}H NMR spectra

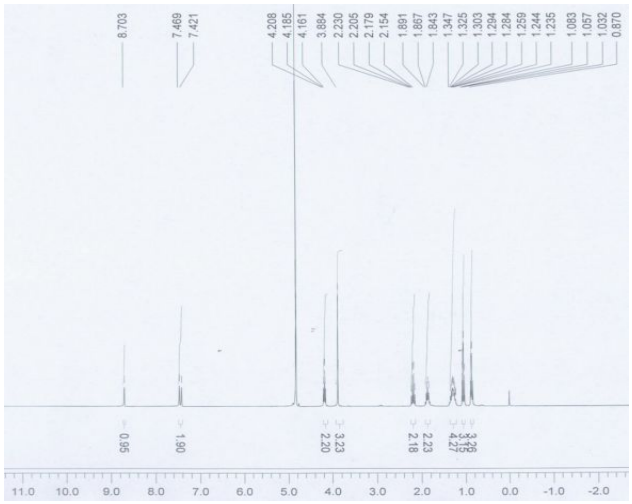

图 S1　离子液体[C_5mim][Pro]的 ^{1}H NMR 谱图

Fig.S1　^{1}H NMR spectrum of the IL [C_5mim][Pro]

表 S1　[C_5mim][Pro]的核磁共振谱表征 δ_H (300 MHz, D_2O)

Table S1　The ^{1}H NMR of [C_5mim][Pro]

Chemical shift	Hydrogen number	Radical
0.870 (t)	3	$NCH_2\ CH_2\ (CH_2\ )_2\mathit{CH_3}$
1.259 (t)	3	$\mathit{CH_3}CH_2COO$
1.347(m)	4	$NCH_2\ CH_2\ \mathit{(CH_2\ )_2}CH_3$
1.891~1.843(m)	2	$NCH_2\ \mathit{CH_2}(CH_2\ )_2CH_3$
2.230~2.154(m)	2	$\mathit{CH_2}COO$
3.884(s)	3	$N\mathit{CH_3}$
4.208~4.161 (t)	2	$N\mathit{CH_2}$
7.421(d)	1	C(4)H
7.469(d)	1	C(5)H
8.703 (s)	1	C(2)H

m: multiple peak; t: three peaks; d: double peak; s: single peak

Section B　DSC measurement

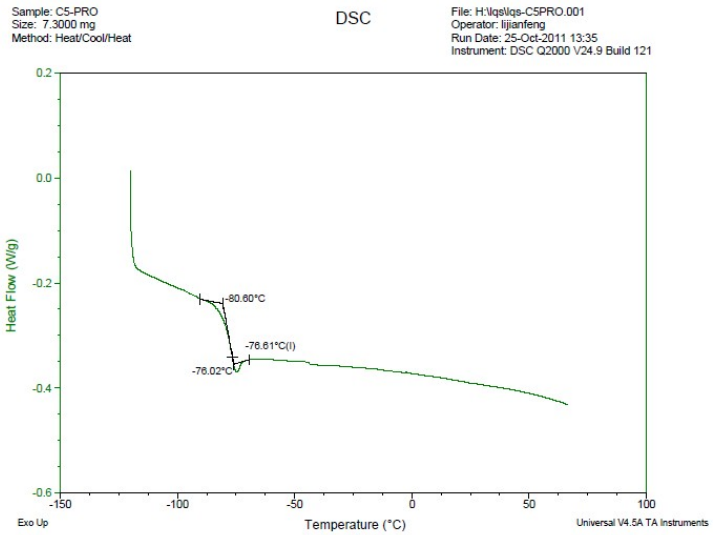

图 S2　离子液体[C_5mim][Pro]的 DSC 图

Fig.S2　DSC trace of IL [C_5mim][Pro]

表 S2　在 288.15-318.15 K 范围内不同浓度的[C_5mim][Pro]水溶液和纯水的热膨胀系数 α/K^{-1}

Table S2　The values of the coefficient of thermal expansion, α/K^{-1}, for aqueous [C_5mim][Pro] with various molalities at 288.15-318.15 K

m/mol·kg^{-1}	T/K						
	288.15	293.15	298.15	303.15	308.15	313.15	318.15
				water			
0	1.16	1.60	2.05	2.50	2.96	3.41	3.87
				aqueous [C_5mim][Pro]			
0.0111	1.684	2.12	2.557	2.997	3.438	3.881	4.327
0.0278	1.701	2.137	2.574	3.012	3.453	3.896	4.341
0.0557	1.736	2.17	2.606	3.044	3.484	3.926	4.370
0.1112	1.810	2.242	2.675	3.109	3.546	3.985	4.427
0.1670	1.853	2.289	2.727	3.167	3.609	4.054	4.501
0.2774	2.087	2.492	2.899	3.307	3.718	4.130	4.545
0.3350	2.201	2.598	2.997	3.397	3.799	4.204	4.611
0.3913	2.306	2.695	3.085	3.477	3.872	4.268	4.667
0.4477	2.404	2.786	3.171	3.558	3.946	4.337	4.730

表 S3　288.15-318.15 K 范围内[C_5mim][Pro]水溶液表观摩尔体积$^{\phi}V_B$的值

Table S3　The values of $^{\phi}V_B$/cm^3·mol^{-1} for the aqueous [C_5mim][Pro] calculated from eq. (4)

m/mol·kg^{-1}	T/K						
	288.15	293.15	298.15	303.15	308.15	313.15	318.15
0.0111	215.7	216.8	217.9	218.2	219.4	220.8	222.1
0.0278	215.3	216.2	217.2	217.8	218.9	220.0	221.2
0.0557	214.7	215.4	216.6	217.4	218.5	219.4	220.6
0.1112	214.0	214.8	215.7	216.7	217.7	218.6	219.6
0.1670	213.4	214.3	215.1	216.2	217.2	218.1	219.1
0.2774	212.3	213.4	214.4	215.3	216.3	217.2	218.0
0.3350	211.8	212.9	214.0	214.8	215.9	216.8	217.7
0.3913	211.7	212.6	213.7	214.6	215.5	216.5	217.4
0.4477	211.3	212.2	213.3	214.3	215.2	216.2	217.1

表 S4　用方程(7)计算得到的溶质的表观摩尔膨胀率ϕ_E的值

Table S4　The values of the apparent molar expansibility of the solute, ϕ_E/cm^3·mol^{-1}·K^{-1}, calculated from eq. (7) for aqueous [C_5mim][Pro]

m/mol·kg^{-1}	T/K						
	288.15	293.15	298.15	303.15	308.15	313.15	318.15
0.0111	0.1488	0.1678	0.1868	0.2058	0.2248	0.2438	0.2628
0.0278	0.1516	0.1654	0.1792	0.1930	0.2068	0.2206	0.2344
0.0557	0.1742	0.1819	0.1896	0.1972	0.2049	0.2126	0.2202
0.1112	0.1765	0.1811	0.1857	0.1904	0.1950	0.1996	0.2042
0.1670	0.1802	0.1838	0.1874	0.1909	0.1945	0.1981	0.2016
0.2774	0.2138	0.2065	0.1992	0.1919	0.1846	0.1774	0.1701
0.3350	0.2121	0.2064	0.2007	0.1950	0.1893	0.1836	0.1778
0.3913	0.2018	0.1989	0.1960	0.1931	0.1902	0.1873	0.1844
0.4477	0.2111	0.2061	0.2011	0.1961	0.1911	0.1861	0.1811

表 S5　利用方程(8)计算得到的ϕ_E(est)的值

Table S5　The values of the apparent molar expansibility of the solute, ϕ_E(est)/cm^3·mol^{-1}·K^{-1}, calculated from eq. (8) for aqueous [C_5mim][Pro]

m/mol·kg^{-1}	T/K						
	288.15	293.15	298.15	303.15	308.15	313.15	318.15
0.0111	0.1534	0.1723	0.1913	0.2103	0.2206	0.2403	0.2602
0.0278	0.1517	0.1651	0.1823	0.1959	0.2062	0.2202	0.2346
0.0557	0.1758	0.1818	0.1899	0.1981	0.2029	0.2114	0.2202
0.1112	0.1766	0.1808	0.1860	0.1905	0.1942	0.1999	0.2048
0.1670	0.1814	0.1842	0.1872	0.1910	0.1937	0.1977	0.2013
0.2774	0.2141	0.2067	0.1993	0.1920	0.1845	0.1774	0.1703
0.3350	0.2128	0.2069	0.2007	0.1949	0.1890	0.1834	0.1776

0.3913	0.2022	0.1989	0.1960	0.1931	0.1901	0.1875	0.1850
0.4477	0.2111	0.2058	0.2007	0.1957	0.1906	0.1860	0.1810

表 S6　将利用工作方程(11)预测的[C_5mim][Pro]离子液体水溶液的表面张力值 γ_{Prd} (mJ·m^{-2})

Table S6　The predicted values of the surface tension, γ_{Prd}(mJ/cm^{-2}), for aqueous [C_5mim][Pro]

m/mol·kg^{-1}	T/K						
	288.15	293.15	298.15	303.15	308.15	313.15	318.15
0.0111	73.1	72.4	71.8	71.1	70.4	69.7	69.1
0.0278	72.7	72.0	71.4	70.7	70.0	69.4	68.7
0.0557	72.1	71.4	70.7	70.1	69.4	68.7	68.1
0.1112	70.8	70.1	69.5	68.8	68.1	67.5	66.8
0.167	69.5	68.9	68.2	67.5	66.8	66.2	65.5
0.2774	67.0	66.3	65.7	65.0	64.3	63.7	63.0
0.335	65.7	65.0	64.4	63.7	63.0	62.3	61.7
0.3913	64.4	63.7	63.1	62.4	61.7	61.1	60.4
0.4477	63.1	62.4	61.8	61.1	60.4	59.8	59.1

表 S7　其余温度下[C_5mim][Pro]水溶液等张比容实验值, P(Exp), 等张比容计算值, P_m, ΔP, 和等张比容预测值, P(Est)

Table S7　The values of the experimental parachor, P(Exp), parachor, P_m ,ΔP, A_p, and P(Est) for the aqueous [C_5mim][Pro] at other temperatures

m/mol·kg^{-1}	288.15 K				298.15 K			
	P	P_m	ΔP	P(Est)	P	P_m	ΔP	P(Est)
0.0111	52.80	52.89	-0.09	52.89	52.69	52.72	-0.03	52.72
0.0278	52.92	53.04	-0.11	52.95	52.83	52.87	-0.04	52.78
0.0557	53.08	53.28	-0.20	53.11	52.97	53.11	-0.14	52.94
0.1112	53.48	53.76	-0.29	53.42	53.37	53.60	-0.23	53.26
0.1670	53.79	54.25	-0.45	53.73	53.68	54.09	-0.41	53.57
0.2774	54.41	55.20	-0.79	54.34	54.28	55.05	-0.77	54.19
0.3350	54.71	55.70	-0.99	54.66	54.51	55.55	-1.03	54.52
0.3913	54.92	56.19	-1.27	54.97	54.78	56.03	-1.25	54.83
0.4477	55.20	56.67	-1.47	55.28	55.07	56.52	-1.46	55.14
A_p		-3.11						
m/mol·kg^{-1}	303.15 K				308.15 K			
	P	P_m	ΔP	P(Est)	P	P_m	ΔP	P(Est)
0.0111	52.62	52.65	-0.03	52.65	52.59	52.59	0.00	52.59
0.0278	52.76	52.80	-0.04	52.71	52.71	52.74	-0.02	52.65
0.0557	52.91	53.04	-0.13	52.87	52.87	52.98	-0.11	52.81
0.1112	53.31	53.53	-0.22	53.18	53.26	53.47	-0.20	53.12
0.1670	53.60	54.02	-0.41	53.50	53.51	53.96	-0.44	53.43

0.2774	54.20	54.98	-0.78	54.12	54.13	54.92	-0.79	54.05
0.3350	54.47	55.48	-1.01	54.44	54.42	55.42	-1.00	54.37
0.3913	54.70	55.97	-1.27	54.75	54.60	55.91	-1.31	54.68
0.4477	54.96	56.46	-1.50	55.06	54.90	56.40	-1.50	55.00
A_p		-3.07				-3.11		

m/mol·kg^{-1}	318.15 K			
	P	P_m	ΔP	P(Est)
0.0111	52.53	52.48	0.05	52.48
0.0278	52.65	52.63	0.02	52.54
0.0557	52.76	52.87	-0.11	52.70
0.1112	53.16	53.36	-0.20	53.01
0.1670	53.49	53.85	-0.36	53.33
0.2774	54.05	54.82	-0.77	53.94
0.3350	54.28	55.32	-1.04	54.27
0.3913	54.50	55.81	-1.32	54.58
0.4477	54.77	56.30	-1.53	54.89
A_p		-3.12		