Ether-linked diamine carboxylate ionic liquid aqueous solution for efficient absorption of SO_2

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^{1}H NMR data of EDPILs:

[BDMAEE][L] ^{1}H NMR (500 MHz, DMSO, 298.2K, TMS)，δ（ppm）:

1.31(3H, m), 2.61(12H, t), 3.63(4H, t), 3.91(4H, t), 4.21(1H, s), 4.82(1H, s), 7.81(1H,s)

[BDMAEE][L]$_2$ ^{1}H NMR (500 MHz, DMSO, 298.2K, TMS)，δ（ppm）: 1.31(6H, m), 2.61(12H, t), 3.63(4H, m), 3.91(4H, m), 4.21(2H, s), 4.82(2H, s), 7.81(2H,s)

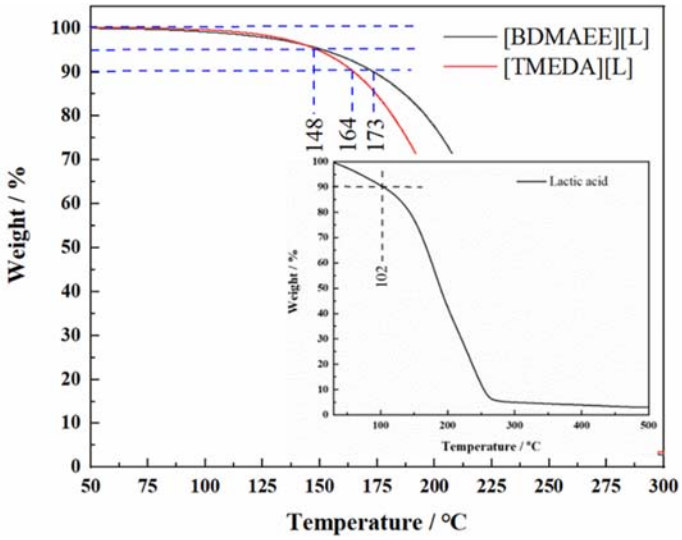


Figure S1. TGA curves of [BDMAEE][L], [TMEDA][L] and lactic acid with a 10 ^{o}C/min temperature heating rate to 800 ^{o}C under the N_2 atmosphere.

We employed a lactic acid of 99.7% purity and 85% content. We further decreased the water content below 6 wt% via evaporation under vacuum before thermal gravimetric analysis was carried out. It was evident that the weight loss before 100 °C was approximately 10 wt%, this may suggest the relatively poor thermal stability of the lactate anion.

Table S1. The water content of the prepared PILs.

PILs	Water contents (wt%)
[TMEDA][L]	0.1030±0.0075

[TMEDA][L]$_2$	0.1244±0.0050
[BDMAEE][L]	0..1156±0.0085
[BDMAEE][L]$_2$	0.1458±0.0060

Quantum chemical calculations. The geometries of the SO_2, BDMAEE, TMEDA, and lactic acid were constructed using GaussView 5.0. To investigate the interaction between PILs and SO_2, SO_2 molecules were added to [BDMAEE][L] or [TMEDA][L] and optimized to obtain the initial structures of PILs-nSO_2 complexes using Molclus software and Gaussian 09 program. Specifically, 500 initial structures of the PILs-nSO_2 complexes were randomly and irregularly engendered using the Genmer tool of the Molclus program. They were then pre-optimized at the PM6 level by using Gaussian 09 program. According to the energy sequence and previous study, several optimized configurations were selected for further density-functional theory (DFT) calculations. Widely used, B3LYP/6-311+G(d,p) computational model was used to conduct all the DFT calculations. Frequency calculations were carried out at the same theoretical level for each optimized complex structures to confirm there was no imaginary frequency. Thus, all the configurations were verified to be local minima. The interaction energy including the basis set superposition errors (BSSE) was determined using the counterpoise method.

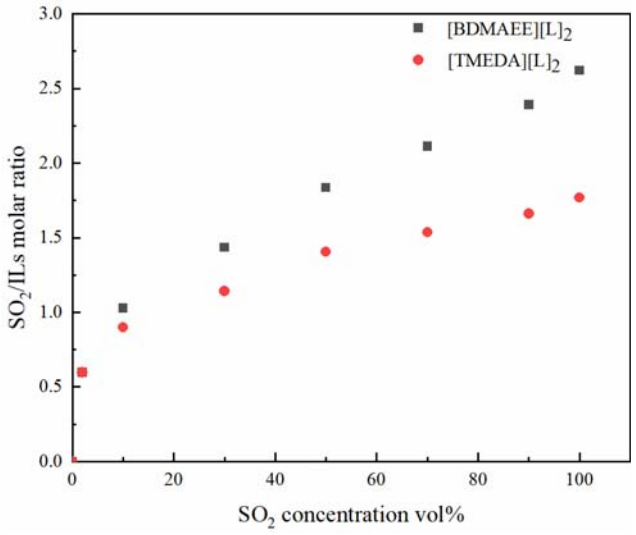
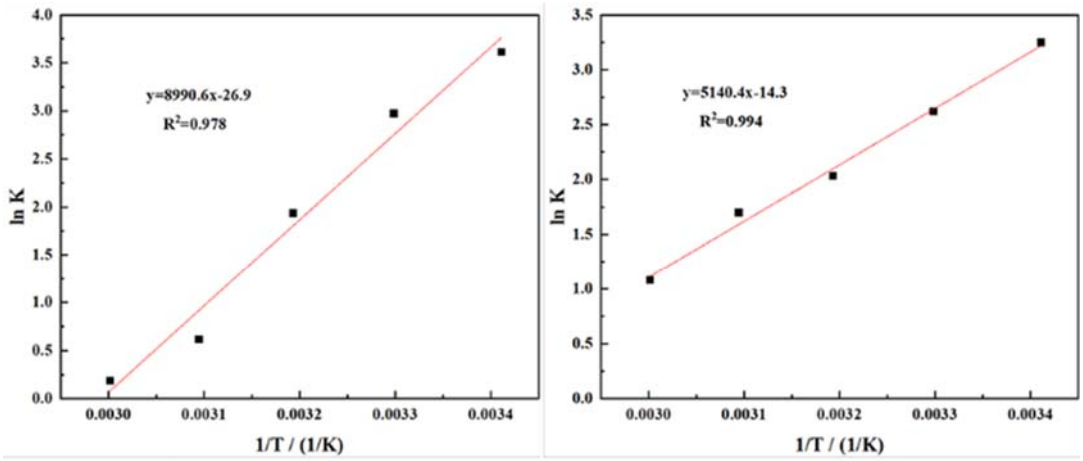


Figure S2. Absorption capacity of SO_2 in $[BDMAEE][L]_2$ and $[TMEDA][L]_2$ with respect to the concentration of SO_2 at 40 °C.

Table S2. The reaction equilibrium constant (K) and related SO_2 absorption experiments data for the absorption enthalpy calculation. (The SO_2 concentration was 100% and the pressure was 1 bar)

$[BDMAEE][L]_2$			$[TMEDA][L]_2$		
T (°C)	Capacity (mol/mol)	K	T (°C)	Capacity (mol/mol)	K
20	2.921	37.119	20	1.925	25.667
30	2.854	19.548	30	1.864	13.706
40	2.621	6.916	40	1.768	7.621
50	1.948	1.853	50	1.690	5.445
60	1.640	1.206	60	1.492	2.937



(a) (b)

Figure S3. The linear relationship between lnK and 1/T for (a) [BDMAEE][L]$_2$ and (b) [TMEDA][L]$_2$.

Physical properties of absorbents. The densities and viscosities of EDPILs aq at 25 °C are listed in Table S2. The properties of the prepared absorbents increased with an increase in lactic acid/diamine ratios and the EDPILs concentrations. Moreover, the viscosities of all studied absorbents ranged from 1.20-6.58 cP, which were significantly lower than those of pure ILs. This indicated that the viscosities of the absorbents could be dramatically decreased via blending EDPILs with water. Conventionally, low viscosities improved the efficiency of heat and mass transfer. Thus it can be deduced that the studied absorbents with low viscosities may have a practical commercial application.

Table S3. Densities and Viscosities of the studied absorbents (25 °C).

ILs aqueous solution	Concentration	Density(g/cm^3)	Viscosity(cP)
[BDMAEE][L] (1:2)	19.6 wt% ILs	1.0376	1.20
[BDMAEE][L] (1:2)	30.1 wt% ILs	1.0557	1.28

[BDMAEE][L] (1:2)	39.9 wt% ILs	1.0738	1.76
[BDMAEE][L] (1:2)	49.8 wt% ILs	1.1235	2.86
[BDMAEE][L] (1:2)	60.3 wt% ILs	1.1348	6.58

Table S4. the SO_2/CO_2 selectivity of $[BDMAEE][L]_2$ aqueous solution (50 wt%)

	mol SO_2 / mol IL		mol CO_2 / mol IL	SO_2 / CO_2 selectivity	
ILs aqueous solution	2 vol %	100 vol %	100 vol %	$S_{0.2/1}$	$S_{1/1}$
$[BDMAEE][L]_2$ aq	1.040	2.815	0.183	5.7	15.4

$S_{0.2/1}$: the molar absorption capasity ratio of 0.2 vol% SO_2 and 100 vol% CO_2 $S_{1/1}$: the molar absorption capasity ratio of 100 vol% SO_2 and 100 vol% CO_2

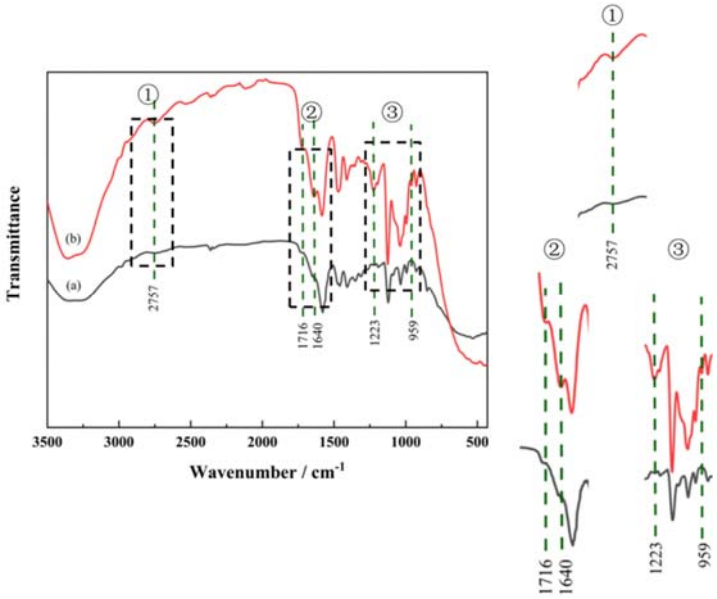


Figure S4. FTIR spectra in detail of 50 wt% $[BDMAEE][L]_2$ aq before (a) and after (b) absorption of SO_2.