Supporting Information

Separation of Taurine and Na_2SO_4 Using in Situ Formation of Deep Eutectic Solvents: Experiments and Computation Simulation

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The identification of present mixture as DES

Based on DSC results, the melting points of Tau/MEA (1:5) DES was 270 K. And the value was expressed in the solid-liquid equilibrium (SLE) diagram as Figure S1. The red lines was obtained by the melting points and $\Delta_{fus}H$ (the enthalpy of fusion) of two pure compounds [1,2]. It can be seen that the melting point of the prepared mixture was lower than the ideal eutectic point represented as $T_{E,\ ideal}$. Therefore, the present mixture can be named as DES according to the broad definition.

The melting point of ideal binary mixture was calculated as following,

$$\frac{1}{T_m} = \frac{1}{T_{m,A}} + \frac{R}{H_{fus,A}} \ln \frac{1}{x_A} \qquad \text{(S1)}$$

Where $T_{m,A}$ is the melting point of pure substance A, $H_{fus,A}$ is the fusion enthalpy of A, x_A is the molar fraction of A, and R is ideal gas constant.

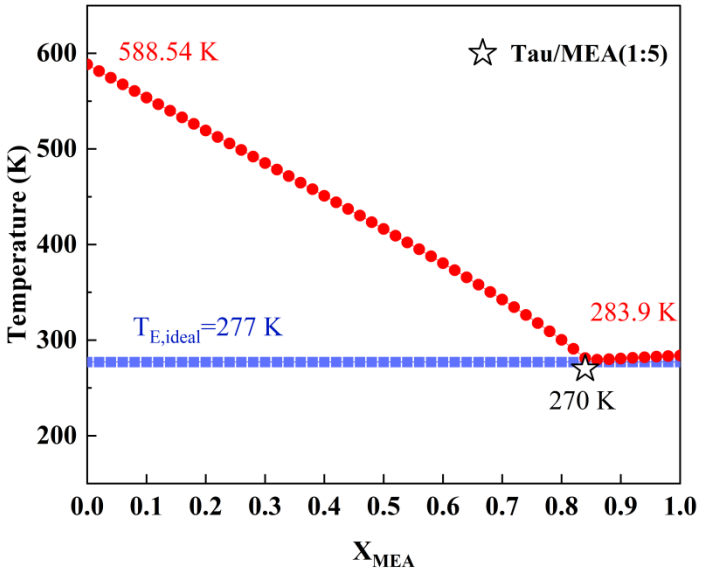

Figure. S1. Melting point and ideal binary solution phase diagram for Tau/MEA (1:5) DES.

[1] X.-W. Han, C.-R. Zhou, X.-H. Shi, Determination of specific heat capacity and standard molar combustion enthalpy of taurine by DSC. J Therm Anal Calorim 2012;109:441-6. https://10.1007/s10973-011-1670-y.

[2] A. Penttilä, P. Uusi-Kyyny, A. Salminen, J. Seppälä, V. Alopaeus, A comprehensive thermodynamic study of heat stable acetic acid salt of monoethanolamine. International Journal of Greenhouse Gas Control 2014;22:313-24. https://doi.org/10.1016/j.ijggc.2013.12.001.

The selectivity parameter between taurine and Na_2SO_4

The selectivity parameter between taurine and Na_2SO_4 was calculated to further demonstrate the effectiveness of the separation strategy, which are defined as follows:

$$S = \frac{m_T}{m_S} \quad \text{(S2)}$$

where m_T and m_S are the solubility of Tau and Na_2SO_4 in the DES, respectively.

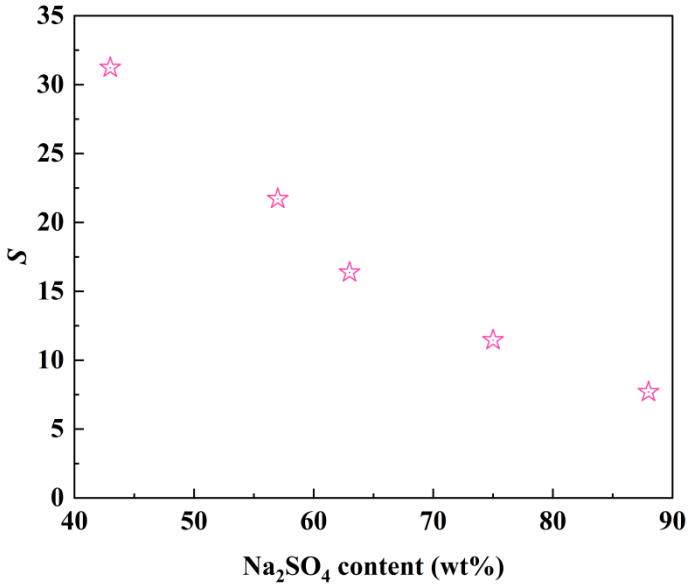

Figure. S2. The selectivity parameter between taurine and Na_2SO_4.

The raw data of Tau yield affected by molar ratio under the condition of Tau:Na_2SO_4 (3:4, mass ratio)

Experiment-1

Molar ratio (Tau:MEA)	Original Tau/g	Recycled Tau/g	Yield%
1:5	3.7459	3.6528	97.51
1:6	3.6720	3.1593	86.04
1:7	3.8438	3.1375	81.62
1:8	4.3676	3.6169	82.81
1:9	3.8245	3.8171	99.08

Experiment-2

Molar ratio (Tau:MEA)	Original Tau/g	Recycled Tau/g	Yield%
1:5	12.3321	12.256	99.38
1:6	3.9715	3.3288	83.82
1:7	3.9171	3.1375	80.10
1:8	3.7206	3.2122	86.33
1:9	3.4922	3.2720	93.69

Experiment-3

Molar ratio (Tau:MEA)	Original Tau/g	Recycled Tau/g	Yield%
1:5	3.7525	3.6479	97.21
1:6	3.7407	3.2073	85.74
1:7	4.1681	3.3919	81.38
1:8	3.8427	3.2221	83.85
1:9	3.5032	3.3690	96.17

Raw data of the experiment affected by Na_2SO_4 content.

Experiment-1

Na_2SO_4 content/wt%	Original Tau/g	Recycled Tau/g	Original Na_2SO_4/g	Removal Na_2SO_4/g
43	3.9132	3.8349	2.9349	2.8121
57	3.5955	3.5329	4.794	4.6340
63	3.3728	2.9046	5.6213	5.4439
75	2.0382	1.3792	6.1146	5.9942
88	1.0767	0.5706	7.5369	7.4627

Experiment-2

Na_2SO_4 content/wt%	Original Tau/g	Recycled Tau/g	Original Na_2SO_4/g	Removal Na_2SO_4/g
43	3.6651	3.5918	2.7488	2.6338
57	3.4876	3.4269	4.6501	4.4950
63	3.0383	2.6166	5.0638	4.9040
75	2.4522	1.6594	7.3566	7.2118
88	1.1696	0.6199	8.1872	8.1067

Experiment-3

Na_2SO_4 content/wt%	Original Tau/g	Recycled Tau/g	Original Na_2SO_4/g	Removal Na_2SO_4/g
43	4.0435	3.9626	3.0326	2.9058
57	3.3369	3.2788	4.4492	4.3008
63	2.8642	2.4666	4.7737	4.6230
75	2.2532	1.5247	6.7596	6.6266
88	1.1729	0.6216	8.2103	8.1295