applied sciences

MDPI

Supporting Information

Study on Degradation of Benzothiazolium-based Ionic Liquids by UV-H_2O_2

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1. Synthesis of Benzothiazole ILs

The benzothiazole hexafluorophosphate IL was synthesized according to the following procedure: 0.05 mol of benzothiazole, 0.05 mol of bromoalkane (CnBr, n=3, 4, 5, 6) and 0.05 mol of potassium hexafluorophosphate are sequentially added to a round bottom flask. The mixture is stirred and refluxed at 90 ℃ to 110 ℃ for 6 h. After cooling to room temperature, a slight excess of dichloromethane was added to the round bottom flask. After stirring and dissolving, the insoluble matter was filtered off. Wash the filtrate with an equal volume of distilled water for 3 to 5 times in a separatory funnel until it did not react with the silver nitrate solution. Dichloromethane was removed by rotary distillation under reduced pressure. The remaining solid was crystallized three times with ethanol. The obtained white needle-like solid was dried in a vacuum oven at 50 ℃ for 24 h. The rest of the IL were synthesized in a similar manner. As the result, the purities of all the investigated ILs were in the range of 96.71-98.66%(See Figure S2).

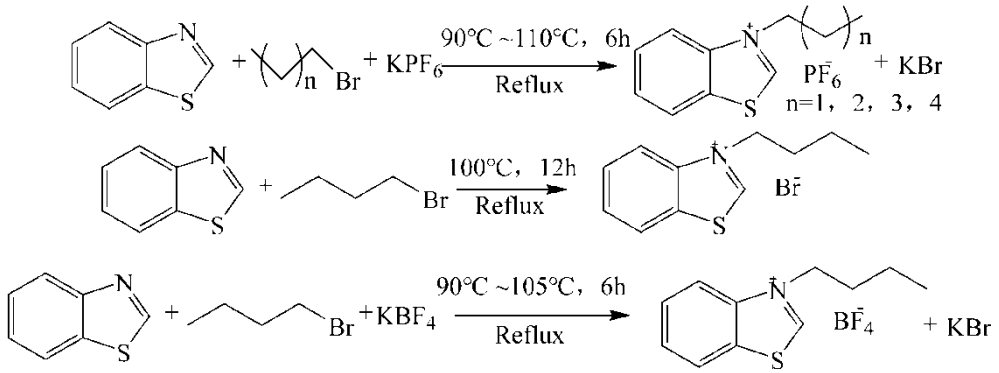

Figure S1. The synthesis procedure of benzothiazole-based ionic liquids.

2. ILs's purity calculation method is the following equation

$$\textit{Ionic liquid purity} = \textit{Peak area of ionic liquid} / \textit{Total peak area} \times 100\ \%, \quad (1)$$

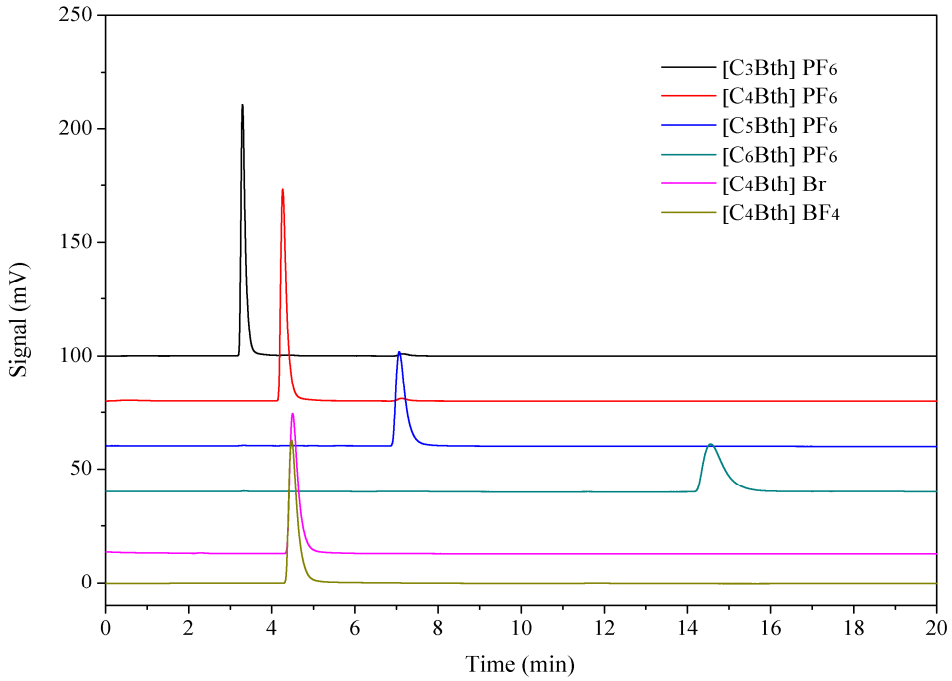

Figure S2. HPLC chromatogram of six benzothiazolium-based ionic liquids.

3. Fitting of kinetic constants

According to figure S3b, we can calculate the kinetic rate constant k corresponding to different concentrations. And this is what is represented in Figure S3c. Finally, we can get the values of b and c_0 according to the fitting equation between ln k and lnc_0.

We perform a regression analysis of the rate constant k and c_0 (0.05-0.20mM) to obtain the relationship between k and c_0.

$$k=k_2 c_0^b, \tag{2}$$

$$lnk=lnk_2+blnc_0, \tag{3}$$

In eq 2, k_2 and b are constants. When c_0 is in the range of 0.05-0.20mM, ln c_0 is plotted on the abscissa and ln k is plotted on the ordinate. Then we can calculate the values of k_2 and b. ($k_2 = e^{-4.9390} = 0.00716$, $b=-0.8063$)

$$k=0.0071c_0^{-.8063}, \tag{4}$$

Other coefficients are calculated similarly.

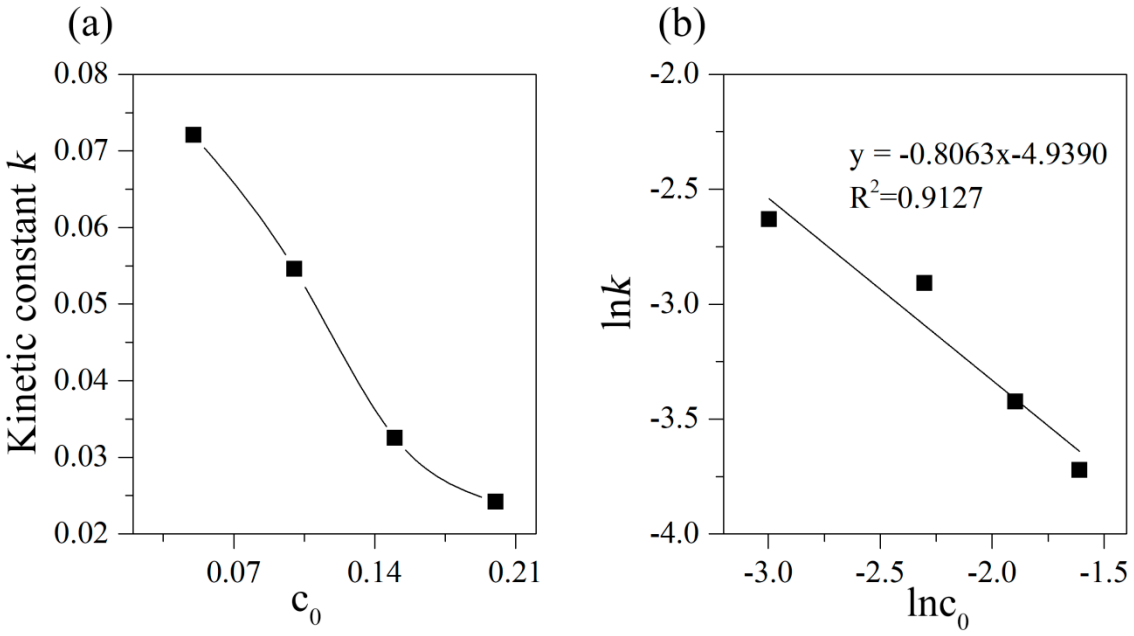

Figure S3. Degradation kinetic constants corresponding to different concentrations of ILs(**a**); Linear fit of *lnk* and lnc_0(**b**).

Table S1. Degradation rate constant k under different conditions

$c_{(H2O2)}$ / mM	50	80	100	120	150	
k / min^{-1}	0.0500	0.0506	0.0562	0.0437	0.0398	
pH	1	3	5	7	9	11
k / min^{-1}	0.0274	0.0293	0.0562	0.0573	0.0419	0.0377
T / ℃	25	35	45	55	65	
k / min^{-1}	0.0427	0.0444	0.0562	0.0450	0.0351	
$c_{(ILs)}$ / M	0.05	0.10	0.15	0.20		
k / min^{-1}	0.0721	0.0562	0.0325	0.0242		
Side chain length	C_3	C_4	C_5	C_6		
k / min^{-1}	0.0351	0.0562	0.0381	0.0492		
$c_{(Cl-)}$ / M	0	0.001	0.01	0.1		
k / min^{-1}	0.0562	0.0370	0.0378	0.0367		