Electronic Supplementary Information

Theoretical Study on the Mechanism of Oxidative-Extractive Desulfurization in Imidazolium-Based Ionic Liquid

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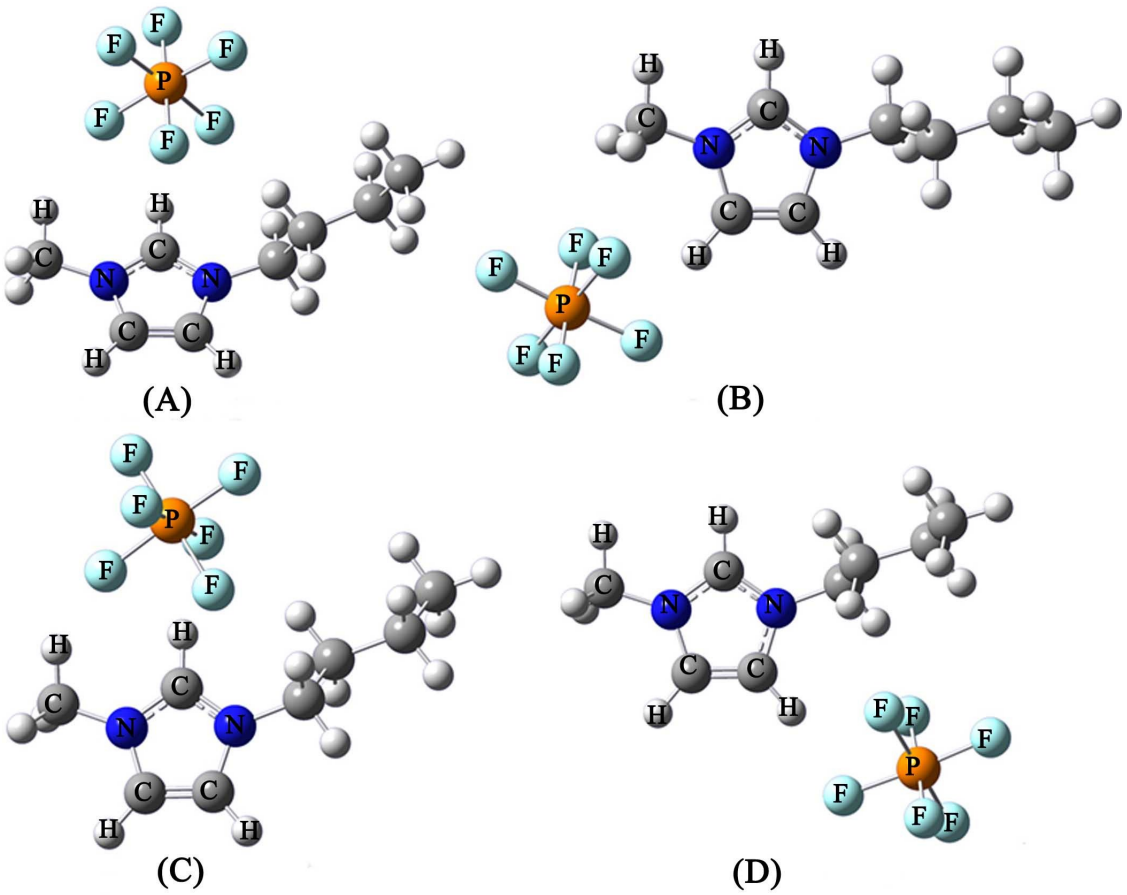

Fig. S1. The different possible structures of [BMIM][PF_6] calculated at B3LYP/6-311++G (d, p) level.

Table S1. The optimized interaction energies of ILs with different alkyl side chains to the imidazolium ring at B3LYP/6-311++G(d, p) level.

	[EMIM][PF_6]		[BMIM][PF_6]			[AMIM][PF_6]	[HMIM][PF_6]
Structure	(A)	(A)	(B)	(C)	(D)	(A)	(A)
ΔE (kJ/mol)	-318.8	-316.9	-283.0	-312.7	-285.6	-316.2	-311.2

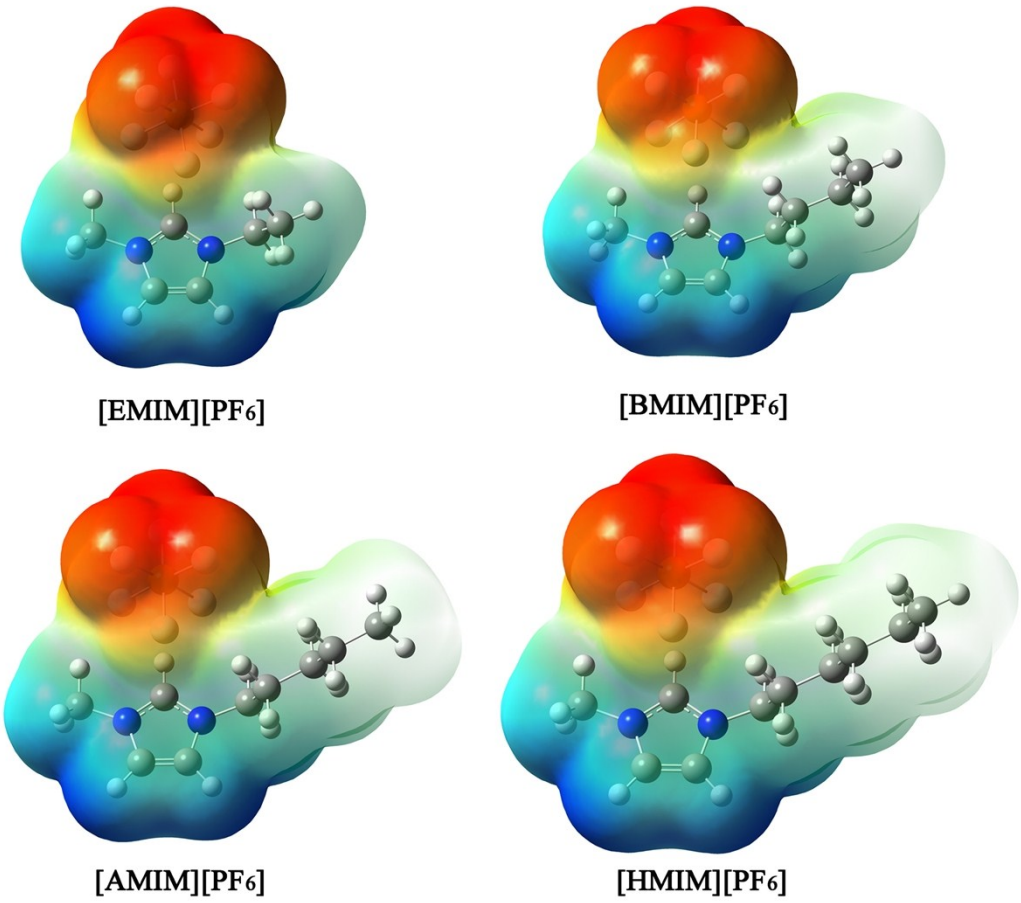

Fig. S2. Electrostatic potential surface of ILs. (The red area represents the negative charge region and the blue area presents the positive charge region and the deeper the color, the greater the charge density.)

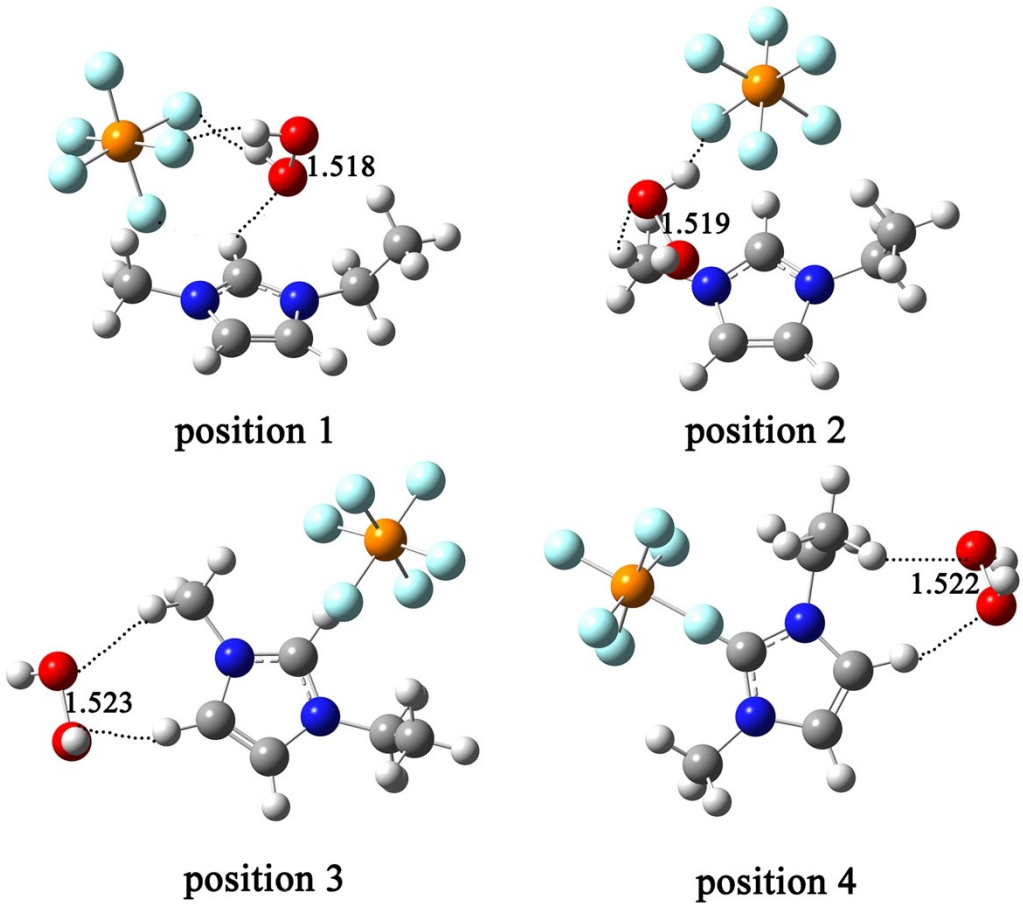

Fig. S3. Four possible geometries of the complex between [EMIM][PF_6] and H_2O_2. Distances of O-O bond are given in angstroms.

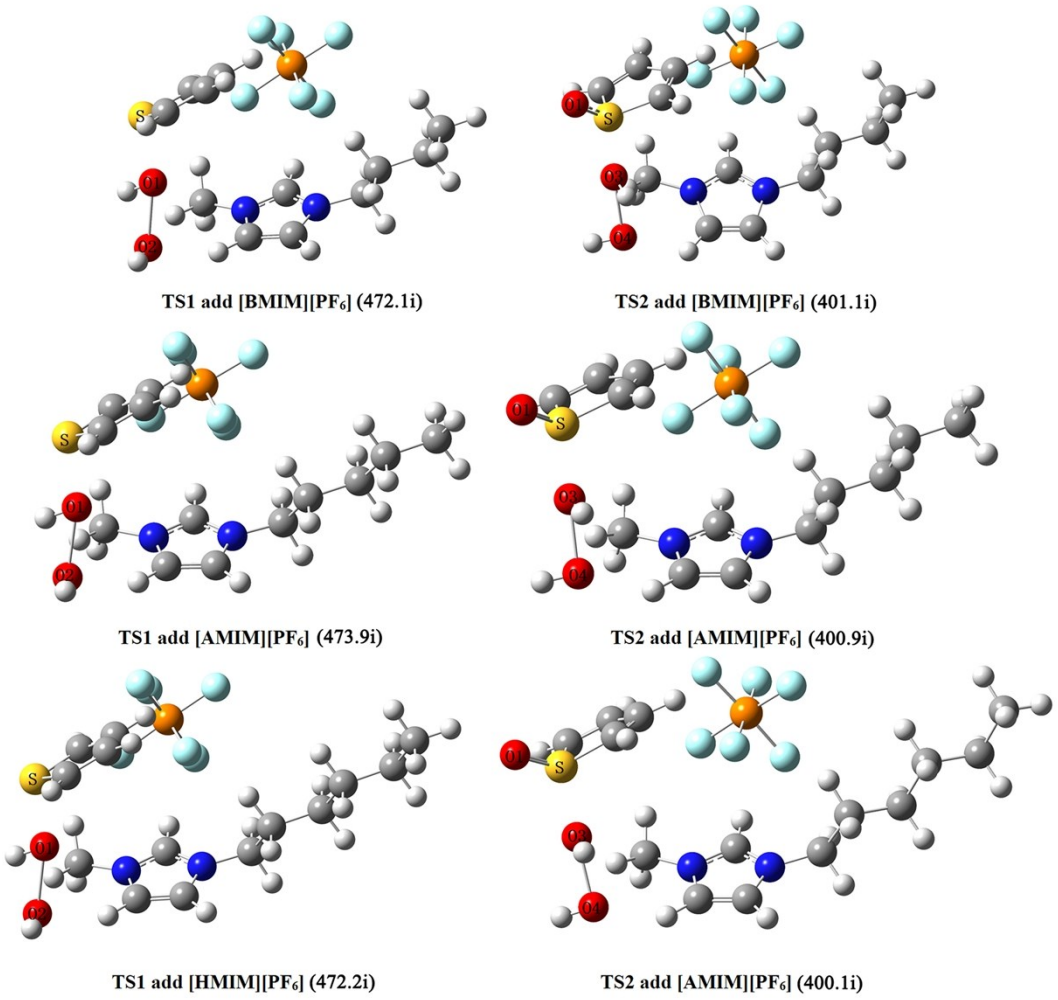

Fig. S4. The transition states for the oxidation process of TH to SP by H_2O_2 in the presence of ILs with different alkyl side chains to the imidazolium ring. The values in parentheses denote the imaginary frequencies of the transition states.