

Microstructures of the Sulfonic-Acid-Functionalized Ionic Liquid/Sulfuric Acid and Their Interactions: A Perspective from the Isobutane Alkylation

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Table S1. Force field parameters for H₂SO₄ molecule.

Atom	Q	σ (nm)	ε (kJ mol ⁻¹)	
Ss	1.080	0.355	0.837100	
Os	-0.440	0.315	0.544000	
O	-0.510	0.315	0.544000	
Hs	0.410	0.010	0.010000	
bond	r_0 (nm)	k_b (kJ mol ⁻¹ nm ⁻²)		
Ss-Os	0.1439	278297		
Ss-O	0.1626	94366		
Hs-O	0.0970	225896		
Bond angle	θ_0 (°)	k_θ (kJ mol ⁻¹ rad ⁻²)		
Ss-O-Hs	109.470	255.204		
Os-Ss-O	105.320	683.158		
Os-Ss-Os	124.570	590.542		
O-Ss-O	101.510	460.543		
	Dihedral coefficient (kJ mol ⁻¹)			
Dihedral	V_1	V_2	V_3	V_4
angle				
Os-Ss-O-Hs	6.275	-0.205	-6.070	0.000
O-Ss-O-Hs	-15.863	-7.797	2.340	0.000

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Table S2. Force field parameters for HSO_4^+ ion.

Atom	Q	σ (nm)	ε (kJ mol ⁻¹)	
Sb	1.364	0.355	0.837100	
Ob	-0.705	0.315	0.544000	
Ob'	-0.649	0.315	0.544000	
O	-0.653	0.315	0.544000	
Hb	0.348	0.010	0.010000	
bond	r_0 (nm)	k_b (kJ mol ⁻¹ nm ⁻²)		
Sb-Ob	0.1480	206566		
Sb-O	0.1714	57124		
Sb-Ob'	0.1470	220693		
Hb-O	0.0965	232339		
Bond angle	θ_0 (°)	k_θ (kJ mol ⁻¹ rad ⁻²)		
Sb-O-Hb	105.010	256.185		
Ob-Sb-Ob	113.794	620.670		
Ob-Sb-O	103.450	595.800		
Ob-Sb-Ob'	115.679	564.880		
O-Sb-Ob'	101.465	518.340		
Dihedral angle	Dihedral coefficient (kJ mol ⁻¹)			
	V_1	V_2	V_3	V_4
Ob-Sb-O-Hb	2.596	1.999	-1.888	-4.060
Ob'-Sb-O-Hb	2.596	1.999	-1.888	-4.060