Study on Hydroxylammonium Based Ionic Liquids. Part II: Computational Analysis of CO_2 Absorption

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Supporting Information

Table S1. Systems and conditions used for molecular dynamics simulations

Number of ion pairs and CO_2 molecules		mole fraction	*T* / K	*P* / MPa	*Name*
[HE3MA]LAC pairs	CO_2	*x* (CO_2)			
125	14	0.1	303	2.5	CO2-01-[HE3MA]
125	31	0.2	303	2.5	CO2-02-[HE3MA]
125	53	0.3	303	2.5	CO2-03-[HE3MA]
125	83	0.4	303	2.5	CO2-04-[HE3MA]
[3HEMA]MS pairs					
125	14	0.1	303	2.5	CO2-01-[3HEMA]
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