

Molecular dynamics and spectroscopic study of sulfur dioxide absorption by an ionic liquid and its mixtures with PEO

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atoms	ϵ (kJ mol ⁻¹)	σ (nm)	q (e)
PEO			
C _z	0,81477	0,37750	0,26500
O _p	0,38452	0,30000	-0,53000
C _p	0,38244	0,39050	0,26500
Cation			
C _n	0,60708	0,39600	0,16800
N _q	0,71175	0,32500	0,32800
C ₁	0,49404	0,39050	-0,06000
C ₂	0,49404	0,39050	0,12700
C ₃	0,49404	0,39050	0,14100
C ₄	0,86666	0,37750	-0,04000
Anion			
C	0,20478	0,35660	0,29880
S	0,80708	0,34200	0,48450
N	0,63844	0,30660	-0,42580
O	0,37945	0,30820	-0,35880
F	0,22285	0,29100	-0,11760
SO₂			
S ₁	0,33900	0,61361	0,59000
O _g	0,30500	0,65684	-0,29500

Tabela S1: Intermolecular parameters

bond	$r(\text{\AA})$	$k_r(\text{kJ mol}^{-1} \text{\AA}^{-2})$
PEO		
C – O	0,1410	267776
C – C	0,1529	224262
Cation		
C – N	0,1471	307105
C – C	0,1529	224262
Anion		
C – S	0,1818	197000
S – N	0,1570	311300
C – F	0,1323	369700
S – O	0,1442	533100
SO₂		
S – O	0,1432	533100

Tabela S2: Intramolecular parameters (bonds)

$$U^i = \sum_{lig} \frac{1}{2} k_r (r - r_{eq})^2$$

Angle	$\theta \text{ (rad)}$	$k_\theta (\text{kJ mol}^{-1} \text{rad}^{-2})$
PEO		
C – O – C	112,0	251,1
O – C – C	112,0	209,1
C – C – O	112,5	209,1
Cation		
C – N – C	113,0	418,4
N – C – C	111,2	669,4
C – C – C	112,7	488,2
Anion		
C – S – N	100,2	816,0
C – S – O	102,6	870,0
S – N – S	125,6	671,0
S – C – F	111,8	694,0
N – S – O	113,6	789,0
O – S – O	118,5	969,3
SO₂		
O – S – O	119,3	460,3

Tabela S3: Intramolecular parameters (angles)

$$U^a = \sum_{ang} \frac{1}{2} k_\theta (\theta - \theta_{eq})^2$$

Dihedral	C_1 (kJ mol ⁻¹)	C_2 (kJ mol ⁻¹)	C_3 (kJ mol ⁻¹)	C_4 (kJ mol ⁻¹)
CNCC	3,04176	-1,35144	0,51881	-2,20915
NCCC	2,92880	-1,46440	0,20920	-1,67360
CCCC	1,71544	2,84512	1,04600	-5,60656

Tabela S4: Intramolecular parameters IL (dihedral)

$$U^d = \sum_{n=0}^4 C_n (\cos \psi)^n$$

Dihedral	C_1 (kJ mol ⁻¹)	C_2 (kJ mol ⁻¹)	C_3 (kJ mol ⁻¹)	C_4 (kJ mol ⁻¹)	C_5 (kJ mol ⁻¹)
CCOC	1,6088	21,2090	-7,8152	-21,4002	6,4267
OCCO	2,2198	17,6174	8,3473	-33,5969	5,0549

Tabela S5: Intramolecular parameters PEO (dihedral)

$$U^d = \sum_{n=0}^4 C_n (\cos \psi)^n$$

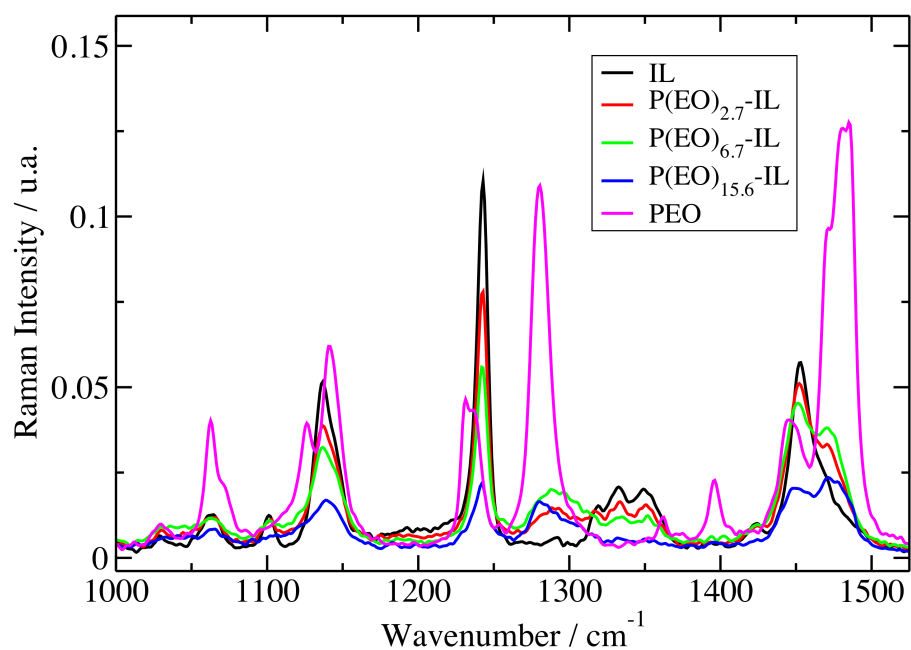


Fig S1. Raman Spectra

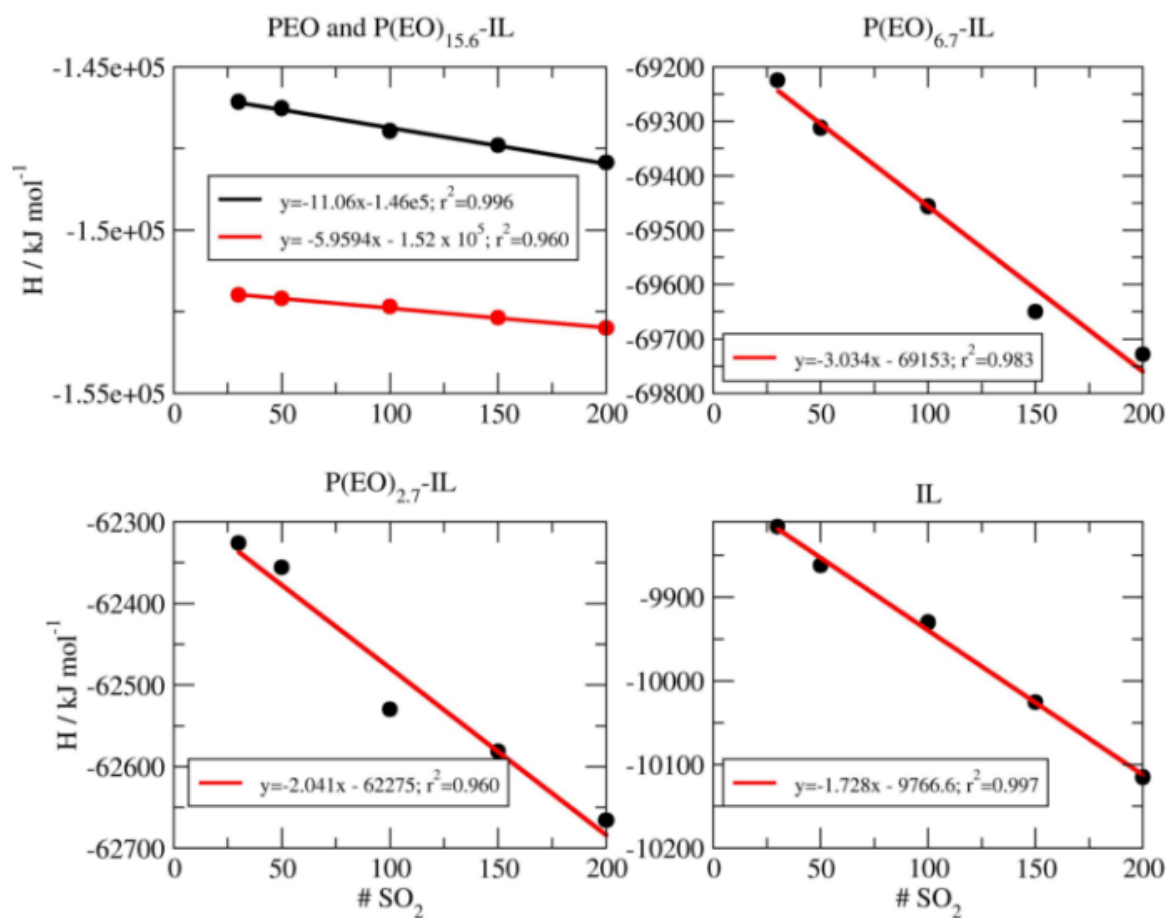


Fig S2: Enthalpy

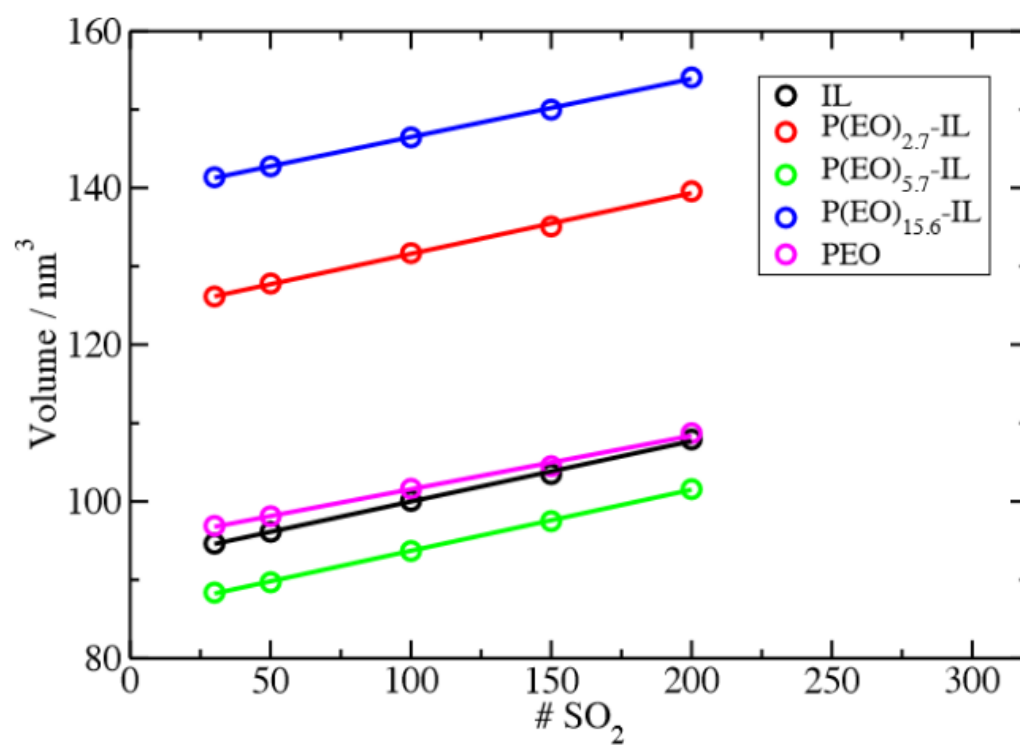


Fig S3: Volume