

Supporting Information

Solubility Properties and Spectral Characterization of Sulfur Dioxide in Ethylene Glycol Derivatives

Shaoyang Sun,^a Yanxia Niu,^{a,b} Zuchen Sun,^a Qiuxia Xu^c and Xionghui Wei^{a*}

^a Department of Applied Chemistry, College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China.

^b College of Chemistry and Chemical Engineering, Taiyuan University of Technology, Taiyuan 030024, China.

^c College of Chemical Engineering, Inner Mongolia University of Technology, Huhhot 010051, China;

*Corresponding authors: Tel/Fax: +86-010-62670662. E-mail: xhwei@pku.edu.cn (X. H. Wei)

Page No.	Contents
S — 2	Fig. S1 Solubility plots of dilute sulfur dioxide in ethylene glycol derivatives at 298.15 K and 122.7 kPa.
S — 3	Fig. S2 Solubility plots of dilute sulfur dioxide in ethylene glycol derivatives at 303.15 K and 122.7 kPa.
S — 4	Fig. S3 Solubility plots of dilute sulfur dioxide in ethylene glycol derivatives at 308.15 K and 122.7 kPa.
S — 5	Fig. S4 Solubility plots of dilute sulfur dioxide in ethylene glycol derivatives at 313.15 K and 122.7 kPa.
S — 6	Fig. S5 Absorption and desorption cycle experiment of SO ₂ in TetraEGDME.
S — 7	Fig. S6 ¹³ C-NMR spectra of DEGDME before and after SO ₂ absorption. (CDCl ₃ as an external reference)
S — 9	Table S1 GLE data of SO ₂ in ethylene glycol derivatives at temperatures ranging from 293.15 K to 313.15 K and a constant total pressure of 122.7 kPa.
S — 10	Table S2 Thermodynamic parameters and Henry's law constants for dilute SO ₂ absorbed in ethylene glycol derivatives at various temperatures at the pressure of 122.7 kPa.

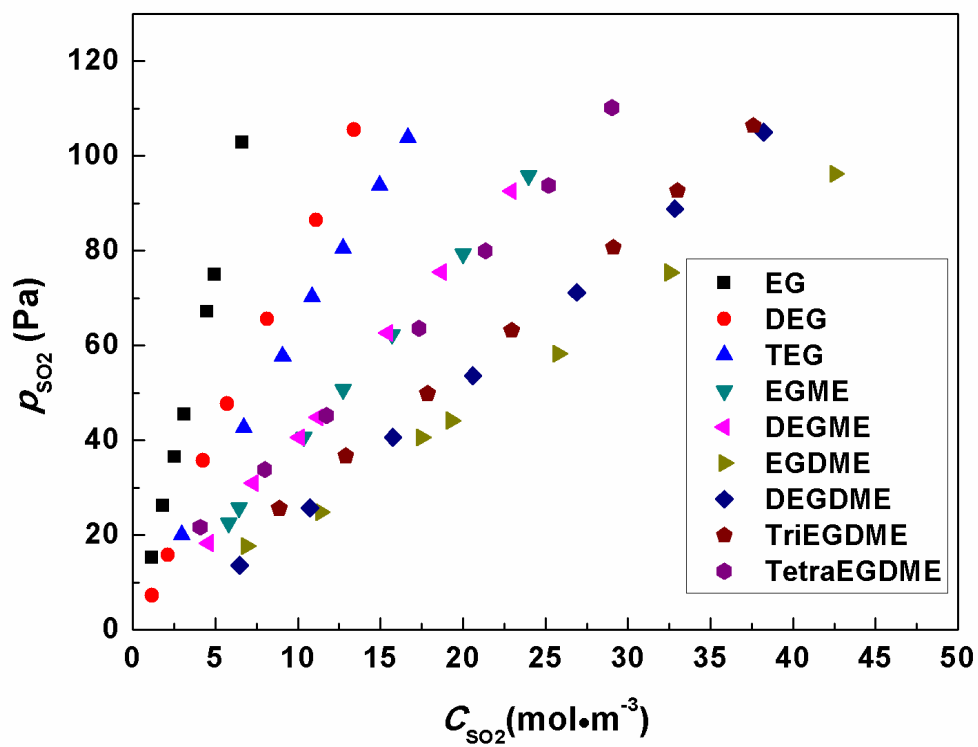


Fig. S1 Solubility plots of dilute sulfur dioxide in ethylene glycol derivatives at 298.15 K and 122.7 kPa.

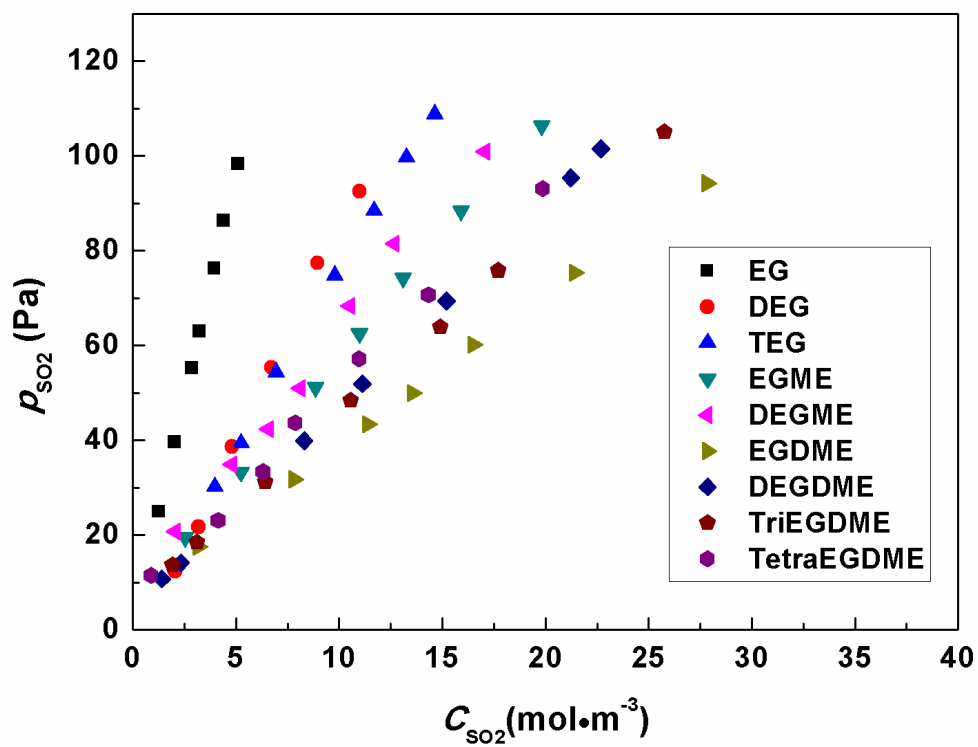


Fig. S2 Solubility plots of dilute sulfur dioxide in ethylene glycol derivatives at 303.15 K and 122.7 kPa.

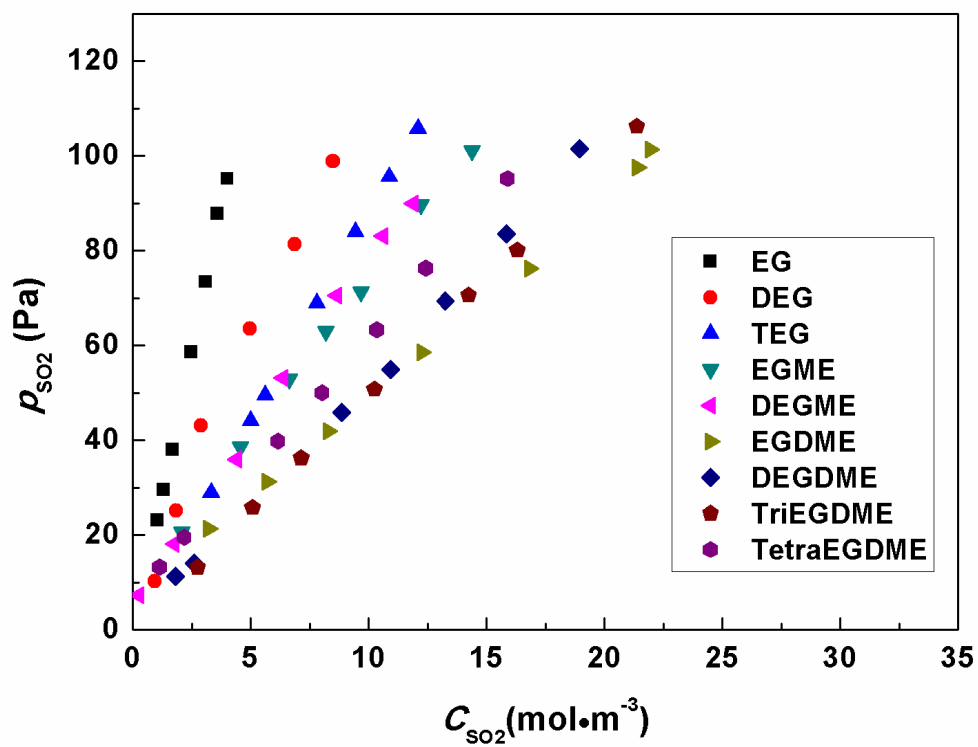


Fig. S3 Solubility plots of dilute sulfur dioxide in ethylene glycol derivatives at 308.15 K and 122.7 kPa.

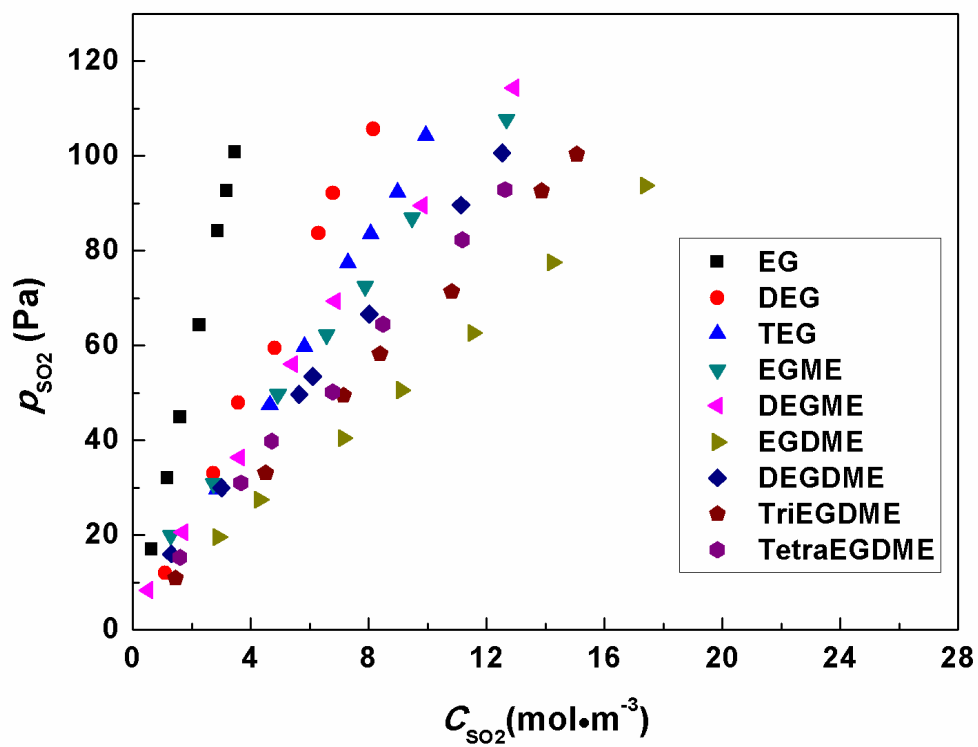


Fig. S4 Solubility plots of dilute sulfur dioxide in ethylene glycol derivatives at 313.15 K and 122.7 kPa.

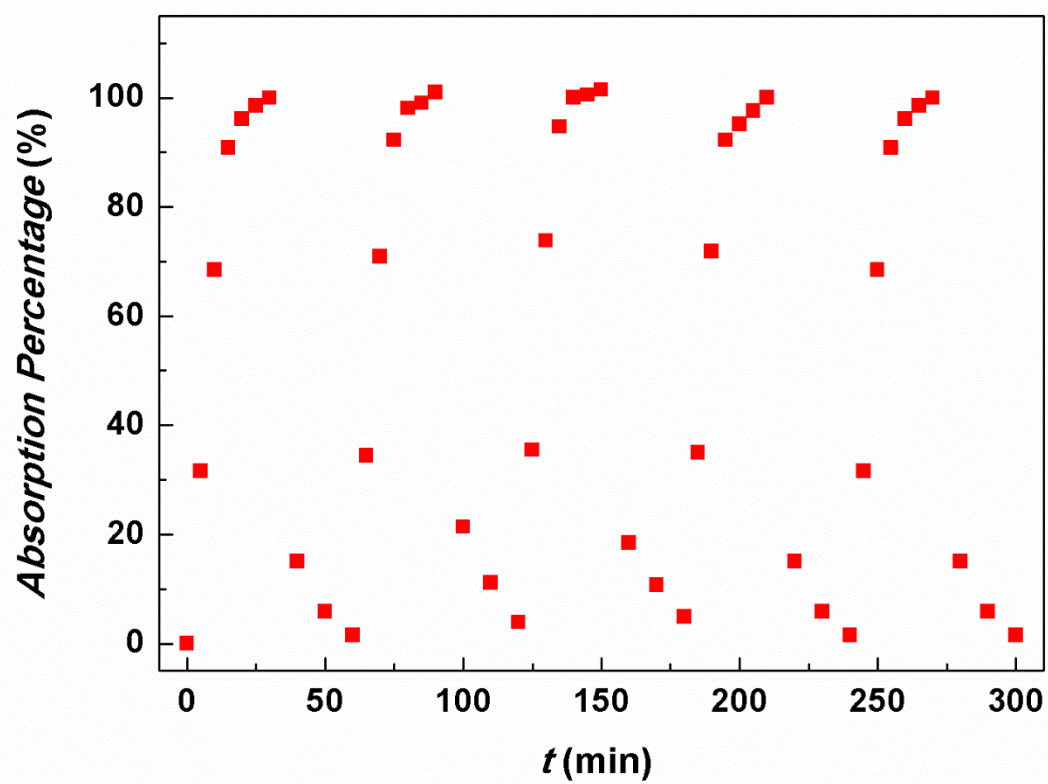


Fig. S5 Absorption and desorption cycle experiment of SO₂ in TetraEGDME.

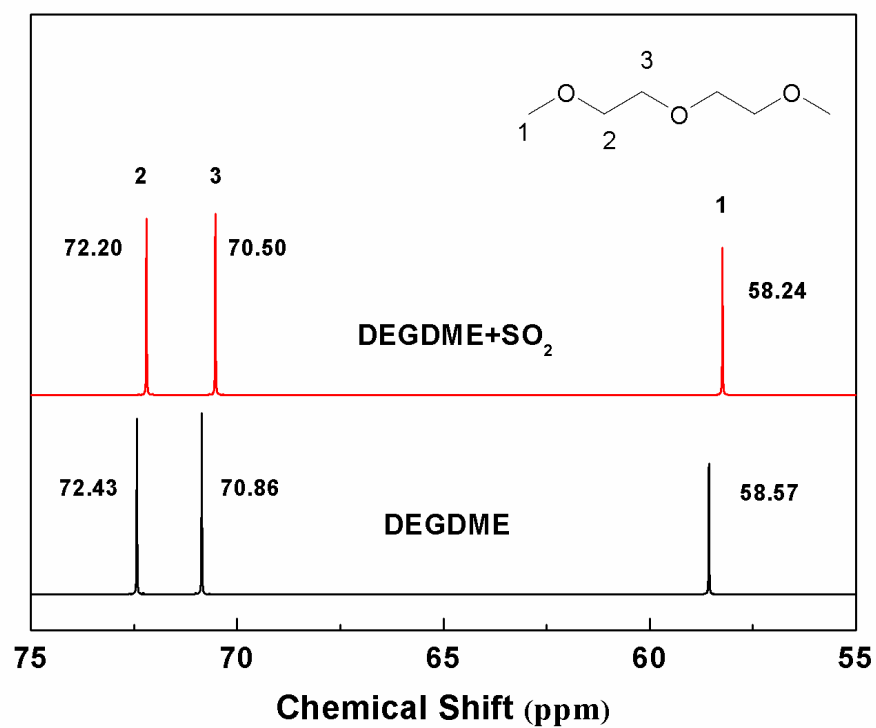


Fig. S6 ¹³C-NMR spectra of DEGDME before and after SO₂ absorption. (CDCl₃ as an external reference)

Table S1 GLE data of SO₂ in ethylene glycol derivatives at temperatures ranging from 293.15 K to 313.15 K and a constant total pressure of 122.7 kPa.

	<i>T</i> =293.15 K		<i>T</i> =298.15 K		<i>T</i> =303.15 K		<i>T</i> =308.15 K		<i>T</i> =313.15 K	
	<i>C</i> _{SO₂}	<i>p</i> _{SO₂}	<i>C</i> _{SO₂}	<i>p</i> _{SO₂}	<i>C</i> _{SO₂}	<i>p</i> _{SO₂}	<i>C</i> _{SO₂}	<i>p</i> _{SO₂}	<i>C</i> _{SO₂}	<i>p</i> _{SO₂}
	(mol·m ⁻³)	(Pa)	(mol·m ⁻³)	(Pa)	(mol·m ⁻³)	(Pa)	(mol·m ⁻³)	(Pa)	(mol·m ⁻³)	(Pa)
EG	1.68	16.9	1.17	15.2	1.26	24.9	1.05	23.1	0.64	16.9
	2.47	26.2	1.84	26.2	2.04	39.6	1.30	29.5	1.17	32.1
	3.63	38.6	2.55	36.4	2.86	55.2	1.68	38.0	1.61	44.9
	4.73	53.9	3.11	45.4	3.24	63.0	2.47	58.6	2.27	64.3
	6.41	73.3	4.49	67.1	3.95	76.2	3.09	73.4	2.88	84.1
	8.10	90.6	4.95	74.9	4.41	86.3	3.60	87.8	3.19	92.6
	10.54	119.8	6.63	102.8	5.10	98.3	4.02	95.2	3.47	100.8
DEG	2.55	20.4	1.16	7.3	2.05	12.3	0.93	10.2	1.09	12.0
	5.30	37.4	2.12	15.7	3.18	21.7	1.83	25.1	2.74	33.1
	9.08	63.3	4.26	35.7	4.80	38.6	2.89	43.1	3.57	47.9
	9.79	68.2	5.70	47.7	6.71	55.4	4.96	63.6	4.81	59.5
	11.88	81.6	8.13	65.5	8.96	77.4	6.87	81.3	6.30	83.6
	13.26	92.8	11.10	86.5	10.98	92.5	8.49	98.9	6.79	92.2
	15.91	110.6	13.40	105.5					8.16	105.7
TEG	1.38	7.4	2.96	20.1	3.98	30.2	3.32	28.9	2.86	29.6
	3.47	21.0	6.73	42.7	5.25	39.4	5.00	44.2	4.64	47.4
	6.27	39.7	9.08	57.7	6.94	54.3	5.61	49.5	5.81	59.7
	9.69	55.5	10.86	70.3	9.79	74.8	7.80	69.0	7.29	77.4
	12.34	70.3	12.75	80.5	11.68	88.4	9.44	84.0	8.06	83.6
	15.81	86.0	14.94	93.8	13.26	99.7	10.86	95.6	8.98	92.3
	19.07	105.1	16.68	103.9	14.64	108.8	12.09	105.7	9.95	104.3
EGME	5.97	17.3	5.81	22.5	2.54	19.4	2.07	20.6	1.29	19.9
	9.28	31.2	6.43	25.8	5.23	33.2	4.55	38.6	2.74	30.8
	11.32	38.2	10.35	40.7	8.85	51.1	6.62	52.9	4.92	49.6
	16.68	54.9	12.75	50.7	10.97	62.5	8.18	63.0	6.57	62.2
	22.95	74.9	15.71	62.3	13.09	74.1	9.68	71.3	7.87	72.4
	28.71	93.6	19.99	79.3	15.89	88.4	12.21	89.7	9.47	86.9
	32.79	104.7	23.97	95.9	19.82	106.3	14.39	101.1	12.68	107.7
DEGME	4.74	17.8	4.59	18.3	2.07	20.7	0.26	7.3	0.52	8.4
	7.65	26.0	7.29	31.0	4.81	34.9	1.76	18.1	1.71	20.6
	11.58	40.6	10.10	40.6	6.57	42.4	4.40	36.0	3.62	36.4
	14.03	51.2	11.22	44.8	8.12	51.0	6.37	53.1	5.43	56.1
	18.51	63.4	15.45	62.6	10.51	68.4	8.64	70.5	6.88	69.4
	21.88	77.1	18.72	75.5	12.68	81.5	10.61	83.1	9.83	89.6
	29.07	98.5	22.95	92.5	17.08	100.9	11.90	90.0	12.94	114.4
EGDME	8.67	16.8	6.89	17.7	3.16	17.5	3.21	21.3	2.90	19.6
	12.39	25.1	11.37	24.8	7.81	31.8	5.69	31.2	4.30	27.4
	19.74	37.6	17.49	40.5	11.39	43.4	8.28	41.9	7.14	40.5
	23.21	43.1	19.28	44.2	13.56	49.9	12.26	58.6	9.11	50.6
	33.66	61.4	25.76	58.3	16.51	60.1	16.82	76.2	11.54	62.6
	42.94	83.8	32.54	75.4	21.42	75.3	21.39	97.5	14.23	77.5

	54.98	104.4	42.53	96.2	27.84	94.3	21.94	101.4	17.39	93.7
	3.72	9.8	6.48	13.5	1.41	10.7	1.81	11.3	1.29	16.0
	12.39	26.6	10.71	25.7	2.31	14.1	2.59	14.0	3.00	30.0
	16.98	39.1	15.76	40.6	8.30	39.9	8.85	45.9	5.64	49.6
DEGDME	20.86	47.4	20.60	53.5	11.12	51.9	10.92	54.9	6.11	53.4
	28.71	65.0	26.88	71.2	15.19	69.4	13.25	69.4	8.02	66.6
	38.20	86.5	32.84	88.9	21.23	95.4	15.84	83.5	11.13	89.6
	42.23	95.5	38.20	105.0	22.69	101.6	18.94	101.5	12.52	100.6
	6.83	16.5	8.87	25.5	1.91	13.6	2.74	13.1	1.45	10.9
	12.95	30.2	12.90	36.6	3.11	18.5	5.07	25.8	4.50	33.1
	18.05	40.8	17.85	49.8	6.42	31.2	7.14	36.2	7.14	49.4
TriEGDME	22.44	52.1	22.95	63.2	10.56	48.4	10.25	50.8	8.38	58.2
	31.31	70.8	29.12	80.7	14.90	63.9	14.23	70.6	10.82	71.3
	35.55	79.6	33.00	92.6	17.70	75.8	16.30	80.1	13.87	92.6
	45.19	102.0	37.59	106.4	25.77	105.1	21.37	106.2	15.06	100.3
	3.77	11.7	4.08	21.7	0.88	11.5	1.14	13.2	1.60	15.3
	7.34	20.9	8.01	33.8	4.14	23.1	2.17	19.5	3.67	31.0
	15.91	45.4	11.73	45.2	6.31	33.4	6.16	39.8	4.71	39.8
TetraEGDME	22.08	59.1	17.34	63.6	7.87	43.7	8.02	50.0	6.78	50.2
	27.23	73.2	21.37	80.0	10.97	57.2	10.35	63.3	8.49	64.5
	32.03	86.5	25.19	93.8	14.33	70.7	12.42	76.3	11.18	82.3
	39.47	102.3	29.02	110.2	19.87	93.1	15.89	95.2	12.63	92.9

Table S2 Thermodynamic parameters and Henry's law constants for dilute SO₂ absorbed in ethylene glycol derivatives at various temperatures at the pressure of 122.7 kPa.

		T/K				
		293.15	298.15	303.15	308.15	313.15
EG	$10^3 H'$	4.76±0.06	6.44±0.06	7.64±0.06	9.65±0.14	11.47±0.09
	$\Delta G/\text{kJ}\cdot\text{mol}^{-1}$	-13.0	-12.5	-12.3	-11.9	-11.6
	$\Delta H/\text{kJ}\cdot\text{mol}^{-1}$			-32.8		
	$\Delta S/\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$			-68.6		
DEG	$10^3 H'$	2.78±0.03	3.19±0.07	3.63±0.07	4.18±0.23	5.20±0.16
	$\Delta G/\text{kJ}\cdot\text{mol}^{-1}$	-14.3	-14.2	-14.2	-14.0	-13.7
	$\Delta H/\text{kJ}\cdot\text{mol}^{-1}$			-23.2		
	$\Delta S/\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$			-29.9		
TEG	$10^3 H'$	2.21±0.06	2.48±0.03	2.94±0.04	3.43±0.03	4.04±0.06
	$\Delta G/\text{kJ}\cdot\text{mol}^{-1}$	-14.9	-14.9	-14.7	-14.5	-14.4
	$\Delta H/\text{kJ}\cdot\text{mol}^{-1}$			-23.3		
	$\Delta S/\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$			-28.3		
EGME	$10^3 H'$	1.32±0.03	1.62±0.01	2.01±0.02	2.56±0.05	3.01±0.06
	$\Delta G/\text{kJ}\cdot\text{mol}^{-1}$	-16.2	-15.9	-15.6	-15.3	-15.1
	$\Delta H/\text{kJ}\cdot\text{mol}^{-1}$			-32.1		
	$\Delta S/\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$			-55.4		
DMGME	$10^3 H'$	1.38±0.03	1.62±0.02	2.19±0.08	2.84±0.06	3.28±0.10
	$\Delta G/\text{kJ}\cdot\text{mol}^{-1}$	-16.0	-15.9	-15.4	-15.0	-14.9
	$\Delta H/\text{kJ}\cdot\text{mol}^{-1}$			-34.9		
	$\Delta S/\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$			-64.2		
EGDME	$10^3 H'$	0.78±0.02	0.91±0.02	1.24±0.01	1.65±0.03	1.96±0.02
	$\Delta G/\text{kJ}\cdot\text{mol}^{-1}$	-17.5	-17.4	-16.9	-16.4	-16.2
	$\Delta H/\text{kJ}\cdot\text{mol}^{-1}$			-37.3		
	$\Delta S/\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$			-67.5		
DEGDME	$10^3 H'$	0.92±0.01	1.16±0.01	1.70±0.01	2.05±0.04	2.86±0.02
	$\Delta G/\text{kJ}\cdot\text{mol}^{-1}$	-17.0	-16.8	-16.1	-15.9	-15.2
	$\Delta H/\text{kJ}\cdot\text{mol}^{-1}$			-43.3		
	$\Delta S/\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$			-89.4		
TriEGDME	$10^3 H'$	0.91±0.01	1.13±0.01	1.53±0.02	1.93±0.01	2.49±0.04
	$\Delta G/\text{kJ}\cdot\text{mol}^{-1}$	-17.1	-16.8	-16.3	-16.0	-15.6
	$\Delta H/\text{kJ}\cdot\text{mol}^{-1}$			-38.8		
	$\Delta S/\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$			-74.1		
TetraEGDME	$10^3 H'$	1.05±0.02	1.43±0.04	1.74±0.05	2.17±0.03	2.66±0.05
	$\Delta G/\text{kJ}\cdot\text{mol}^{-1}$	-16.7	-16.2	-16.0	-15.7	-15.4
	$\Delta H/\text{kJ}\cdot\text{mol}^{-1}$			-34.7		
	$\Delta S/\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$			-61.7		