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Supplementary Material

Table S1 The FAC, diffusion coefficients of VOCs, and g(r) for the intermolecular interactions occurred between C atom of VOCs and S atom of sulfate in the aqueous dual VOCs-sulfate systems. The g(r) values were obtained from **Figure S13**.

Models	VOCs	FAC (%)	g(r) C1（or specific C on Aromatics)			C2		C3	C4	C5	C6	C7	C'(sub C)	Tg	*D* (10^{-4} cm^2/s)	total FAC	Tg (system)
ethylbenzene & 1-methylcyclopentene	ethylbenzene	5.4	0.74	0.98	1.17								1.17	4.06	1.03	10.40	7.58
	1-methylcyclopentene	5	0.33	0.42		0.20	0.41	0.56	0.50	0.32			0.78	3.52	1.55		
toluene & p-xylene	toluene	5.4	0.49	0.72	0.98								2.34	4.53	0.75	7.00	7.41
	p-xylene	1.6	1.44	3.08	3.76								3.24	2.88	0.57		
p-xylene & ethylbenzene	p-xylene	1.6	0.96	2.16	3.08								2.22	2.11	0.49	7.00	5.34
	ethylbenzene	5.4	0.52	0.74	0.98								0.99	3.23	0.51		
ethane & toluene	ethane	0	0.42											0.42	2.55	5.40	5.31
	toluene	5.4	0.86	1.02	1.24								1.77	4.89	0.90		
benzene & methyl cyclohexane	benzene	2	3.60	6.42	6.90									2.82	1.09	4.70	6.34
	methyl cyclohexane	2.7	0.28			1.48	0.84	0.48					0.72	3.52	1.69		
p-xylene & methyl cyclopentane	p-xylene	1.6	1.36	3.20	4.00								3.48	3.01	0.56	1.77	4.15
	methyl cyclopentane	0.17						0.60					0.54	1.14	1.75		
ethane & methyl cyclopentane	ethane	0	0.72											0.72	2.65	0.17	2.29
	methyl cyclopentane	0.17						0.88					0.69	1.57	1.39		

[a]C1 represents number 1 carbon of non-aromatics according to its locant, or the aromatic carbon closest to sulfate. [b]C'(subC) represents carbon on the methyl group of VOCs. The g(r) values presented in the table were calculated from the original values in **Figure S13** using the rules as follows. For aromatics with symmetry, the g(r) values of its specific C were calculated by multiplying the original valid g(r) by the symmetry number, because there are more than one specific C for these VOCs. And g(r) values of the alkyl carbons were estimated by multiplying the original valid g(r) by H number on each -CH_n group. Finally, the Tg values were calculated using the rules as described in the paper.

Table S2 The FAC, diffusion coefficients of VOCs, and g(r) for the intermolecular interactions occurred between C atom of VOCs and S atom of sulfate in the dry dual VOCs-sulfate systems. The g(r) values were obtained from **Figure S12**.

Models	VOCs	FAC (%)	g(r) C1 (or specific C on Aromatics)			C2		C3	C4	C5	C6	C7	C'(subC)	Tg	*D* (10^{-4} cm^2/s)	total FAC	Tg (system)
ethylbenzene & 1-methylcyclopentene	ethylbenzene	5.4	0.89	0.96	1.14								1.50	4.49	0.98	10.40	8.12
	1-methylcyclopentene	5	0.36	0.42		0.22	0.41	0.64	0.38	0.30			0.90	3.63	1.79		
toluene & p-xylene	toluene	5.4	0.62	0.83	1.04								1.44	3.93	0.64	7.00	6.21
	p-xylene	1.6	1.16	2.24	3.20								2.52	2.28	0.46		
p-xylene & ethylbenzene	p-xylene	1.6	1.36	2.56	3.28								3.00	2.55	0.42	7.00	5.76
	ethylbenzene	5.4	0.60	0.64	0.92								1.05	3.21	0.55		
ethane & toluene	ethane	0	0.66											0.66	3.52	5.40	5.83
	toluene	5.4	0.93	1.03	1.26								1.95	5.17	0.52		
benzene & methyl cyclohexane	benzene	2	4.26	6.60	6.60									2.91	1.46	4.70	6.12
	methyl cyclohexane	2.7	0.28			0.88		0.92	0.50				0.63	3.21	3.03		
p-xylene & methyl cyclopentane	p-xylene	1.6	2.16	3.96	4.64								4.74	3.88	0.33	1.77	4.21
	methyl cyclopentane	0.17											0.33	0.33	1.32		
ethane & methyl cyclopentane	ethane	0	0.60											0.60	2.39	0.17	1.56
	methyl cyclopentane	0.17											0.96	0.96	1.55		

[a] C1 represents number 1 carbon of non-aromatics according to its locant, or the aromatic carbon closest to sulfate. [b] C'(subC) represents carbon on the methyl group of VOCs. The g(r) values presented in the table were calculated from the original values in **Figure S12** using the rules as follows. For aromatics with symmetry, the g(r) values of its specific C were calculated by multiplying the original valid g(r) by the symmetry number, because there are more than one specific C for these VOCs. And g(r) values of the alkyl carbons were estimated by multiplying the original valid g(r) by H number on each -CH_n group. Finally, the Tg values were calculated using the rules as described in the paper.

Table S3 The regression statistics for the dry and aqueous dual VOCs-sulfate models.

		dry dual VOCs-sulfate model	R Square	0.96	aqueous dual VOCs-sulfate model	R Square	0.95
			Standard Error	1.28		Standard Error	1.41
			FAC = 1.15 Tg - 0.48 D			FAC = 1.13 Tg - 0.60 D	
	FAC (total) (%)	Predicted 5.4	Residuals	Standard Residuals	Predicted 5.4	Residuals	Standard Residuals
toluene & p-xylene	7	6.64	0.36	0.35	7.60	-0.60	-0.52
p-xylene & ethylbenzene	7	6.18	0.82	0.78	5.45	1.55	1.35
ethane & toluene	5.4	4.79	0.61	0.59	3.94	1.46	1.27
benzene & methyl cyclohexane	4.7	4.91	-0.21	-0.20	5.52	-0.82	-0.71
p-xylene & methyl cyclopentane	1.77	4.06	-2.29	-2.20	3.31	-1.54	-1.34
ethane & methyl cyclopentane	0.17	-0.10	0.27	0.26	0.16	0.01	0.01

Table S4 The FAC, distances (r) and intensities (g(r)) for the S(SO_4^{2-})-O(H_3O^+) and S(SO_4^{2-})-O(H_2O) interactions in the aqueous mono VOC-sulfate systems. The g(r) values were obtained from **Figure S14** and **Figure S15**.

VOCs	FAC (%)	r (S(SO_4^{2-})-O(H_3O^+))	r (S(SO_4^{2-})-O(H_2O))	g(r) (S(SO_4^{2-})-O(H_3O^+))	g(r) (S(SO_4^{2-})-O(H_2O))
toluene	5.4	3.41	3.51	19.1	7.28
ethylbenzene	5.4	3.41	3.37	18.85	4.48
o-xylene	5	3.41	3.49	18.42	9.52
p-xylene	1.6	3.37	3.43	18.84	10.43
benzene	2	3.41	3.41	18.34	9.95
phenol	5	3.39	3.39	18.73	6.05
1-methylcyclopentene	5	3.39	3.39	18.39	10.26
methyl cyclopentane	0.17	3.41	3.43	18.77	8.7
methyl cyclohexane	2.7	3.43	3.45	18.27	9.06
1-heptene	2	3.43	3.53	18.68	9.89
n-heptane	0.06	3.39	3.41	18.64	9.53
ethane	0	3.37	3.39	18.16	8.74
acetylene	0	3.41	3.47	17.73	8.93
dichloromethane		3.39	3.43	18.53	11.4

Table S5 The FAC, distances (r) and intensities (g(r)) for the C(VOC)-O(H_3O^+) interactions in the aqueous mono VOC-sulfate systems. The g(r) values were obtained from **Figure S17**.

VOCs	FAC (%)	r									g(r)								
		C1	C2	C3	C4	C5	C6	C7	[a]C'(subC)	[b]C''	C1	C2	C3	C4	C5	C6	C7	[a]C'(subC)	[b]C''
toluene	5.4	4.77	3.83	3.91	3.73				3.83		0.79	0.74	0.92	0.98				0.83	
ethylbenzene	5.4	4.79	4.09	3.71	3.73				3.95	4.31	0.70	0.70	0.94	1.05				0.64	0.71
o-xylene	5	3.71	3.83	3.79					3.89		0.54	0.80	1.03					0.76	
p-xylene	1.6	4.71	3.69						3.77		0.79	0.72						1.04	
benzene	2	3.77									0.94								
phenol	5	3.77	3.87	4.17	4.45						1.89	1.34	0.76	0.59					
1-methylcyclopentene	5	4.87	3.91	3.93	4.21	3.91			3.87		0.50	0.41	0.50	0.47	0.40			0.56	
methyl cyclopentane	0.17	4.93	4.03	4.61					3.79		0.56	0.40	0.46					0.46	
methyl cyclohexane	2.7	5.05	4.07	4.47	4.63				3.85		0.47	0.33	0.37	0.41				0.42	
1-heptene	2	3.81	4.11	4.35	4.83	4.99	4.75	4.19			0.69	0.58	0.56	0.51	0.47	0.48	0.51		
n-heptane	0.06	3.87	4.73	5.01	5.13						0.49	0.46	0.42	0.43					
ethane	0	3.77									0.35								
acetylene	0	3.51									0.87								
dichloromethane		4.23									1.27								

[a]C'(subC) represents carbon on the methyl group of VOCs, [b]C'' represents the methylene carbon of ethylbenzene.

Table S6 The FAC, distances (r) and intensities (g(r)) for the C(VOC)-O(H_2O) interactions in the aqueous mono VOC-sulfate systems. The g(r) values were obtained from **Figure S16**.

VOCs	FAC (%)	r									g(r)								
		C1	C2	C3	C4	C5	C6	C7	[a]C'(subC)	[b]C''	C1	C2	C3	C4	C5	C6	C7	[a]C'(subC)	[b]C''
toluene	5.4	4.99	3.97	3.91	3.81				4.21		9.98	7.14	10.28	12.30				8.76	
ethylbenzene	5.4	5.51	3.85	3.97	3.63				4.11	4.63	5.14	3.55	4.83	5.63				4.16	4.55
o-xylene	5	5.13	3.89	3.75					3.99		10.19	10.60	14.61					9.10	
p-xylene	1.6	4.91	4.17						4.19		9.30	6.05						8.74	
benzene	2	4.19									7.59								
phenol	5	1.37	2.41	3.67	4.17						2598.87	498.44	230.39	171.38					
1-methylcyclopentene	5	4.81	3.69	4.27	5.13	5.97			3.97		5.31	4.23	4.63	4.52	4.63			5.60	
methyl cyclopentane	0.17	5.03	5.91	5.73					4.27		2.27	1.98	1.99					2.10	
methyl cyclohexane	2.7	5.01	6.13	4.55	4.73				3.69		6.64	5.52	4.96	5.72				5.41	
1-heptene	2	3.83	4.53	5.31	5.77	5.89	4.93	4.15			8.26	6.86	6.10	5.99	5.52	6.11	6.36		
n-heptane	0.06	4.09	4.95	5.19	5.81						3.96	4.06	4.05	4.04					
ethane	0	4.47									1.21								
acetylene	0	3.87									4.23								
dichloromethane		3.51									13.43								

[a]C'(subC) represents carbon on the methyl group of VOCs, [b]C'' represents the methylene carbon of ethylbenzene.

Table S7 The regression statistics for the dry and aqueous mono VOC-sulfate models.

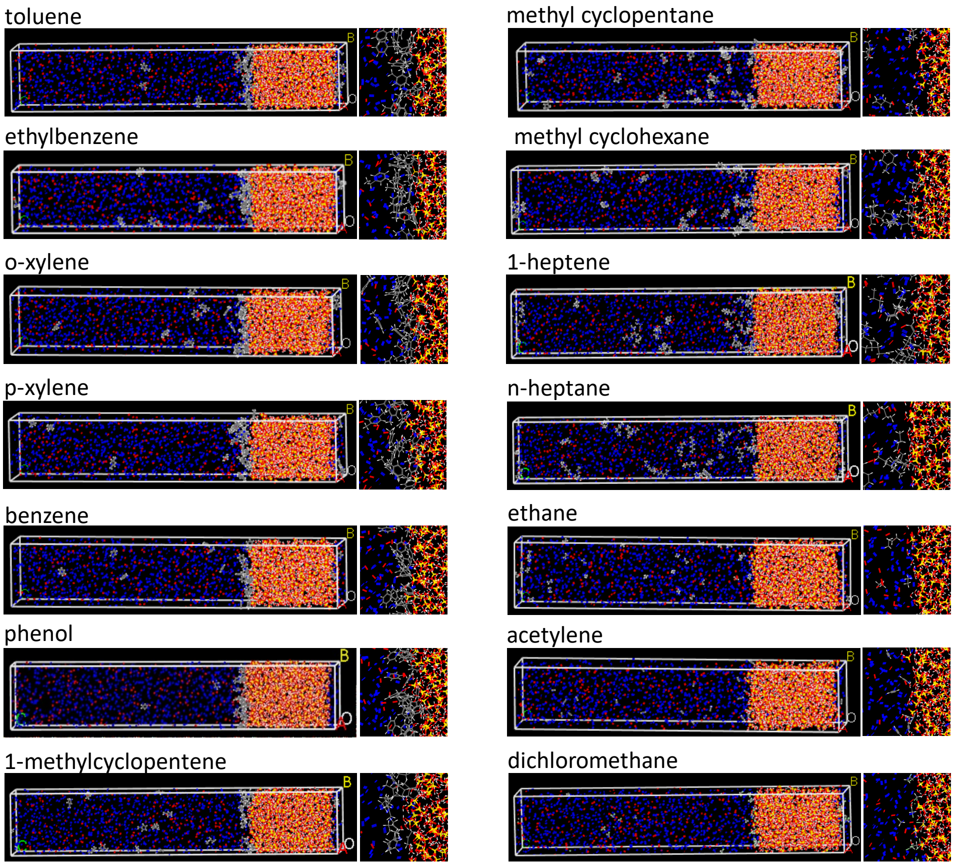
		dry mono VOC-sulfate model	R Square	0.92	aqueous mono VOC-sulfate model	R Square	0.94
			Standard Error	1.00		Standard Error	0.85
			FAC = 0.94 Tg - 0.50 *D*			FAC = 1.00 Tg - 0.62 *D*	
	FAC (%)	Predicted 5.4	Residuals	Standard Residuals	Predicted 5.4	Residuals	Standard Residuals
ethylbenzene	5.4	3.94	1.46	1.60	4.25	1.15	1.47
o-xylene	5	4.03	0.97	1.06	4.17	0.83	1.07
p-xylene	1.6	3.03	-1.43	-1.57	3.20	-1.60	-2.06
benzene	2	2.60	-0.60	-0.66	2.15	-0.15	-0.19
phenol	5	4.08	0.92	1.01	5.30	-0.30	-0.39
1-methylcyclopentene	5	4.93	0.07	0.08	4.13	0.87	1.12
methyl cyclopentane	0.17	0.41	-0.24	-0.26	-0.14	0.31	0.40
methyl cyclohexane	2.7	3.13	-0.43	-0.47	3.19	-0.49	-0.63
1-heptene	2	3.49	-1.49	-1.63	2.88	-0.88	-1.14
n-heptane	0.06	0.26	-0.20	-0.22	0.80	-0.74	-0.95
ethane	0	-0.94	0.94	1.03	-0.20	0.20	0.26
acetylene	0	0.52	-0.52	-0.57	-0.34	0.34	0.43

Table S8 The FAC, diffusion coefficients (*D*) and g(r) for the intermolecular interactions occurred between C atom of VOCs and S atom of sulfate in the aqueous mono VOC-sulfate systems. The g(r) values were obtained from **Figure S11**.

VOCs	FAC (%)	*D* (10^{-4} cm^2/s)	g(r)											
			[a]C1 (or specific C on Aromatics)			C2		C3	C4	C5	C6	C7	[b]C'(subC)	Tg
toluene	5.4	1.40	0.81	1.02	1.15								1.56	4.54
ethylbenzene	5.4	0.64	1.03	1.00	1.08								1.53	4.64
o-xylene	5	0.50	1.64	1.98	2.38								2.94	4.47
p-xylene	1.6	0.66	1.88	4.00	4.40								4.14	3.61
benzene	2	1.14	3.24	6.78	7.08									2.85
phenol	5	0.40	2.85	1.18	1.51									5.54
1-methylcyclopentene	5	1.52	0.47	0.69		0.38	0.58	0.74	0.66	0.46			1.08	5.06
methyl cyclopentane	0.17	1.64											0.87	0.87
methyl cyclohexane	2.7	1.16	0.39			0.88		1.20	0.62				0.81	3.90
1-heptene	2	1.15	0.56	0.69		0.59	0.67					1.08		3.59
n-heptane	0.06	2.03	2.04											2.04
ethane	0	2.77	1.50											1.50
acetylene	0	2.64	0.64	0.65										1.29
dichloromethane		0.17	1.18	1.22	1.14									3.54

[a]C1 represents number 1 carbon of non-aromatics according to its locant, or the aromatic carbon closest to sulfate. [b]C'(subC) represents carbon on the methyl group of VOCs.

The g(r) values presented in the table were calculated from the original values in **Figure S11** using the rules as follows. For aromatics with symmetry, the g(r) values of its specific C were calculated by multiplying the original valid g(r) by the symmetry number, because there are more than one specific C for these VOCs. And g(r) values of the alkyl carbons were estimated by multiplying the original valid g(r) by H number on each -CH_n group. Finally, the Tg values were calculated using the rules as described in the paper.



toluene

ethylbenzene

o-xylene

p-xylene

benzene

phenol

1-methylcyclopentene

methyl cyclopentane

methyl cyclohexane

1-heptene

n-heptane

ethane

acetylene

dichloromethane

Figure S1 The snapshots of the dry mono VOC-sulfate models after the production MD simulation runs and the enlarged views of the snapshots on the surface of sulfate, in which, the pictures to the left are the snapshots of the models and the corresponding enlarged views are next to them. In the snapshots, the left part is air comprising of O_2, N_2 and VOC molecules, and the right yellow part is sulfate and H_3O^+.

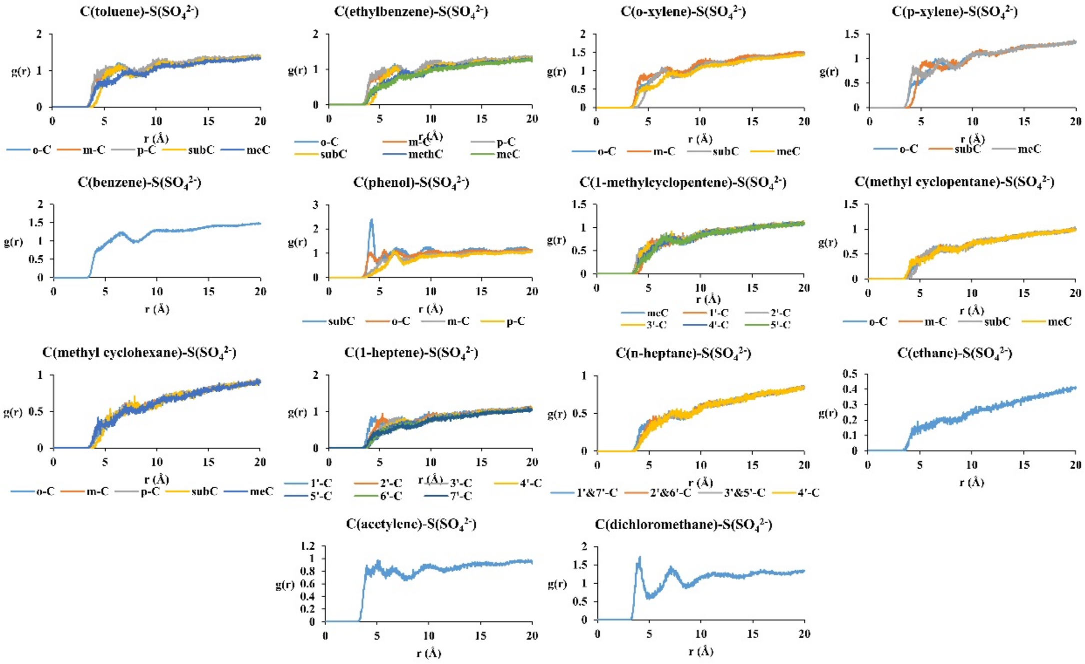


Figure S2 The RDFs for the intermolecular interactions between C atoms of VOCs and S atoms of sulfate in the dry mono VOC-sulfate systems. o-C, m-C, p-C, subC, meC represent the ortho, meta, para, substituted and methyl carbon of VOCs, respectively. H("numeric'"-C) represents the carbon atom at the corresponding locant.

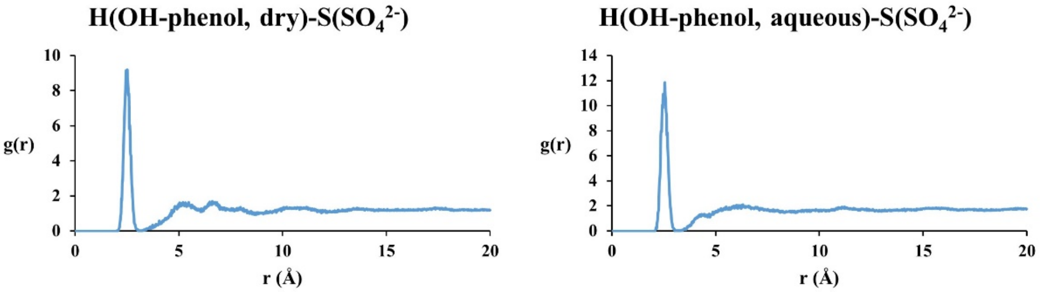
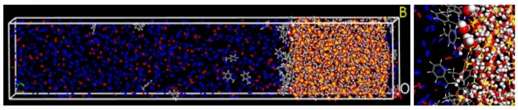
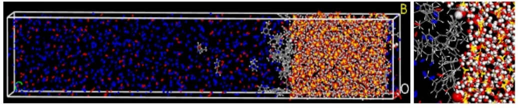


Figure S3 The RDFs for the intermolecular interactions between H atom of OH group of phenol and S atoms of sulfate in the dry and aqueous mono VOC-sulfate systems.

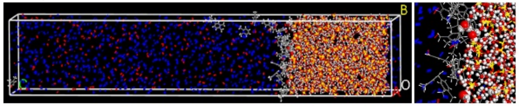
toluene



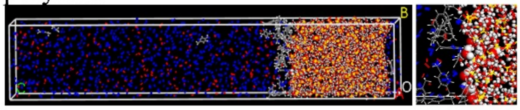
ethylbenzene



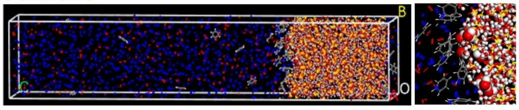
o-xylene



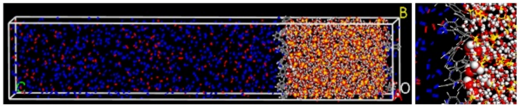
p-xylene



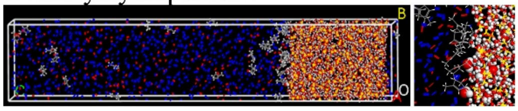
benzene



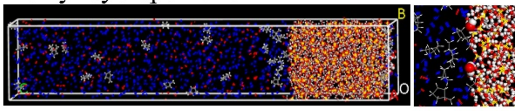
phenol



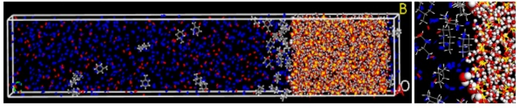
1-methylcyclopentene



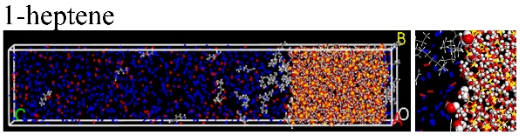
methyl cyclopentane



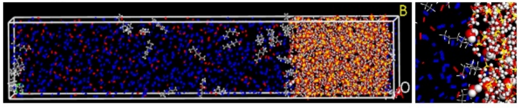
methyl cyclohexane



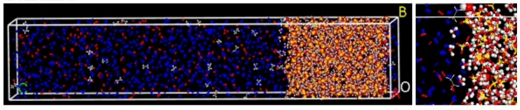
1-heptene



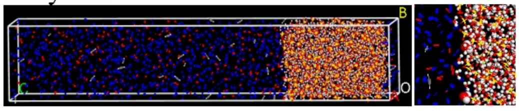
n-heptane



ethane



acetylene



dichloromethane

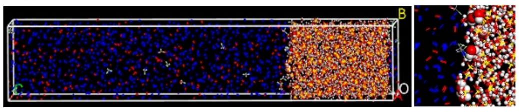


Figure S4 The snapshots of the aqueous mono VOC-sulfate models after production MD simulation runs and the enlarged views of the snapshots on the surface of sulfate, in which, the pictures to the left are the snapshots of the models and the corresponding enlarged views are next to them. In the snapshots, the left part is air comprising of O_2, N_2 and VOC molecules, and the right yellow part is sulfate, H_2O and H_3O^+. From the enlarged views, the big red-white spheres represent H_2O molecules, while the smaller red-white spheres represent H_3O^+ molecules.

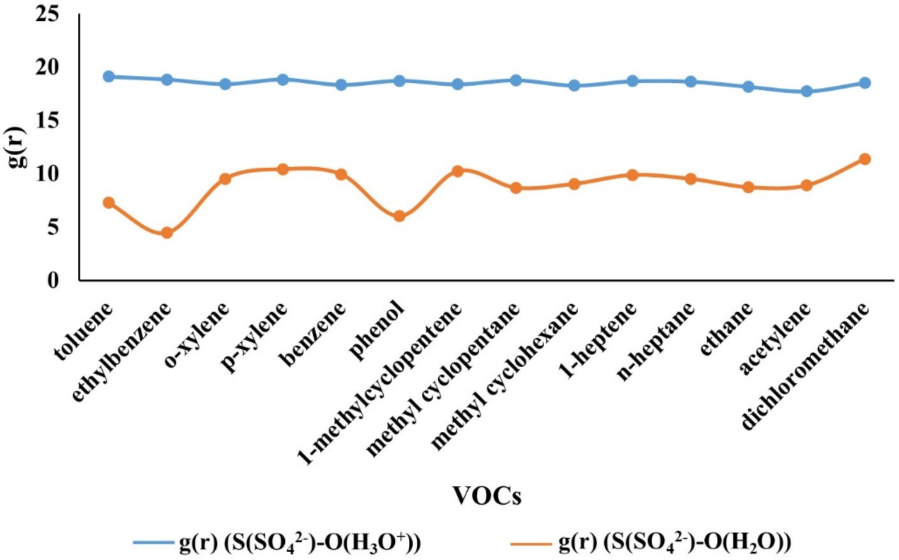


Figure S5 The g(r) of VOCs for the $S(SO_4^{2-})$-$O(H_3O^+)$ and $S(SO_4^{2-})$-$O(H_2O)$ interactions.

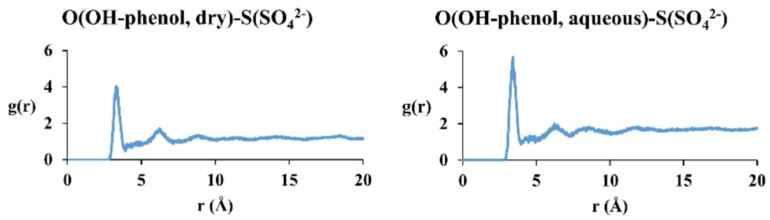


Figure S6 The RDFs for the intermolecular interactions between O atom of phenol and S atoms of sulfate in the dry and aqueous mono VOC-sulfate systems.

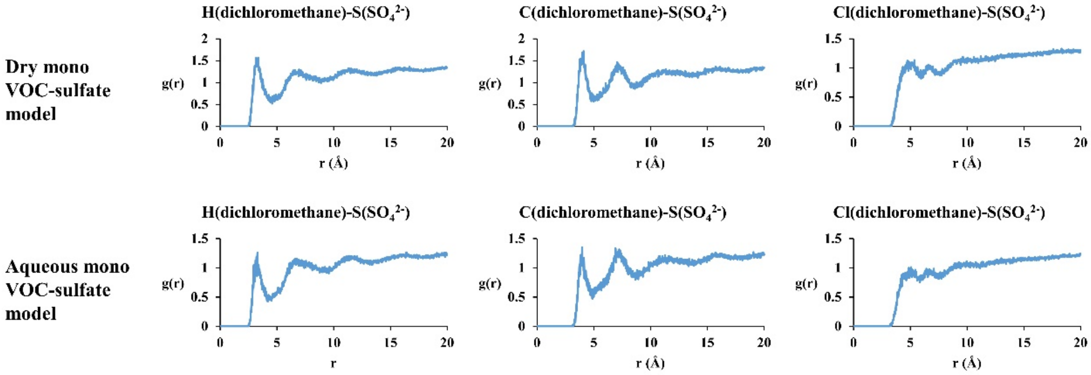


Figure S7 The RDFs for the intermolecular interactions between H, C, Cl atom of dichloromethane and S atoms of sulfate in the dry and aqueous mono VOC-sulfate systems.

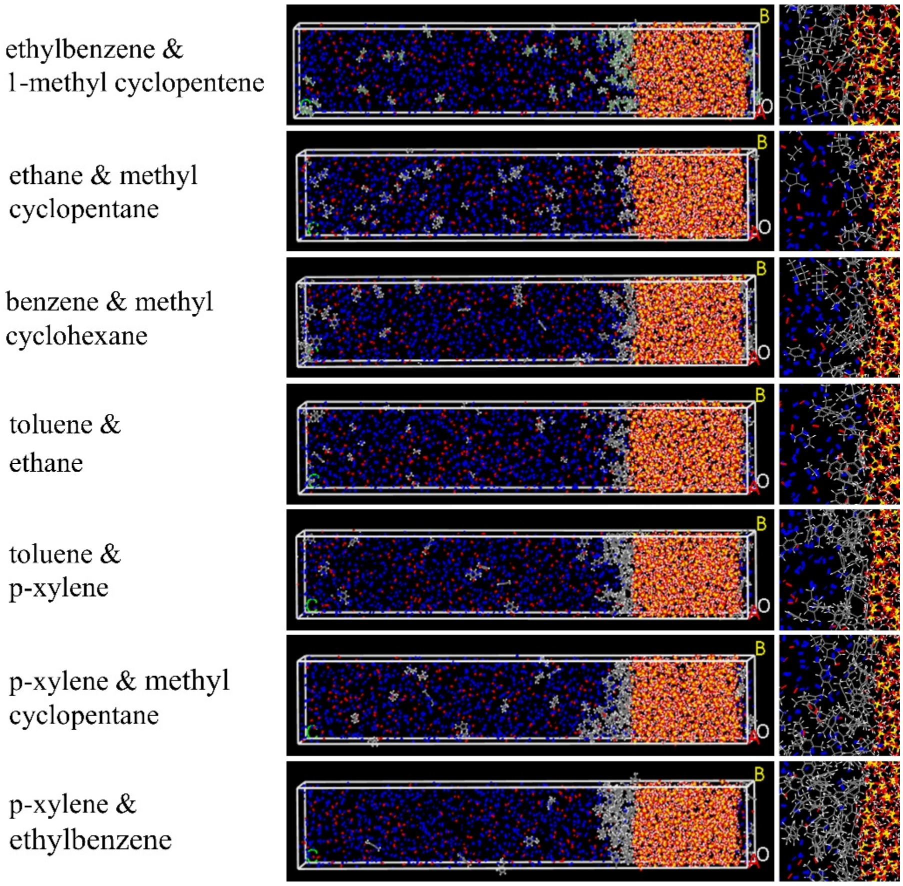


Figure S8 The snapshots of the aqueous dual VOCs-sulfate models after production MD simulation runs and the enlarged views of the snapshots, in which, the pictures to the left are the snapshots of the atmospheric models and the corresponding enlarged views are next to them. In the snapshots, the left part is air comprising of O_2, N_2 and VOC molecules, and the right yellow part is sulfate, H_2O and H_3O^+.

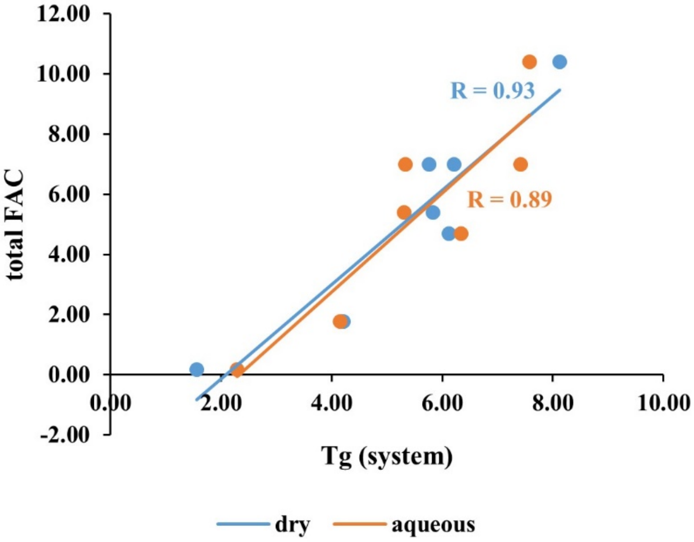
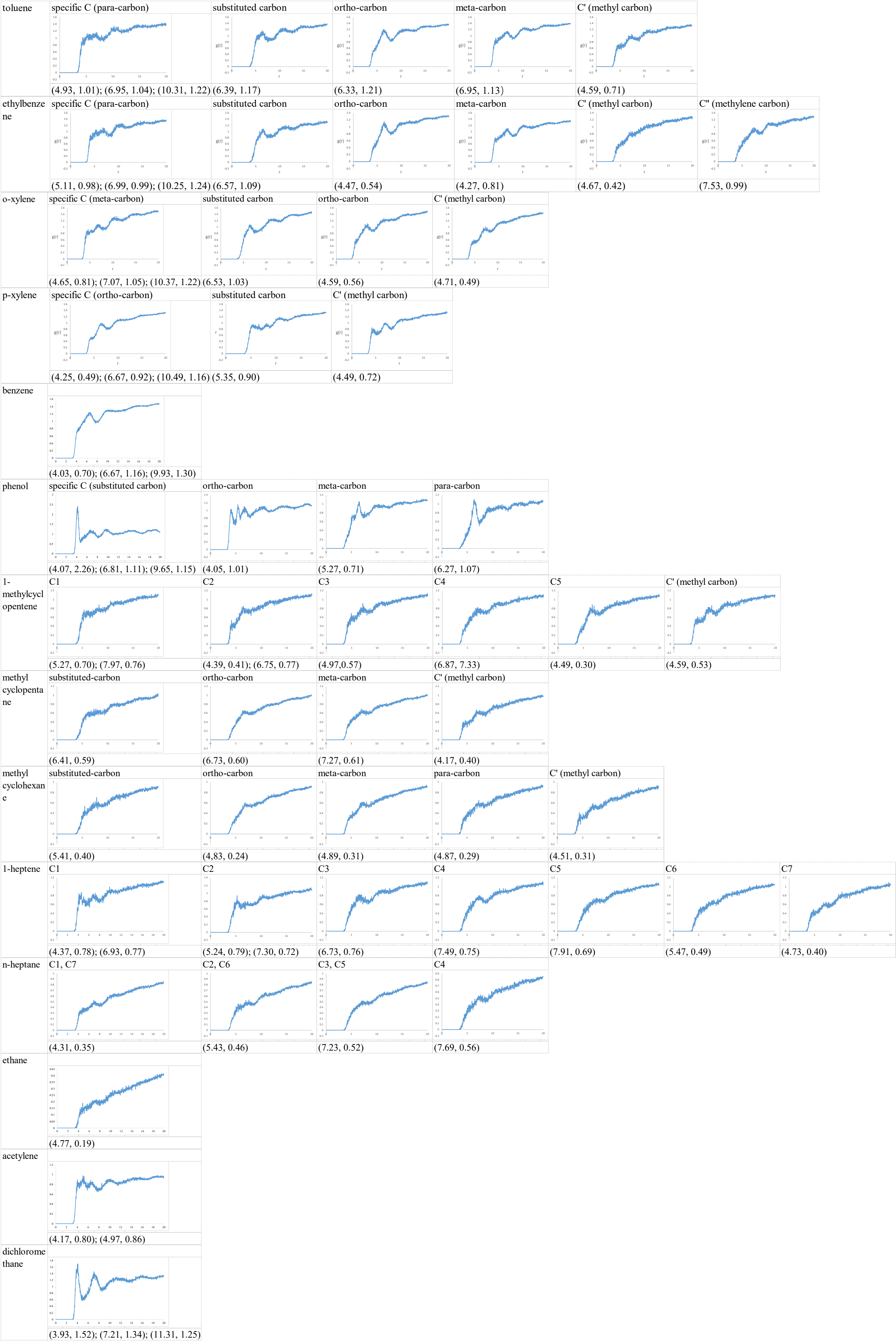


Figure S9 The Tg of each system in the dry and aqueous dual VOCs-sulfate systems as a function of FAC were plotted.



toluene	specific C (para-carbon) (4.93, 1.01); (6.95, 1.04); (10.31, 1.22)	substituted carbon (6.39, 1.17)	ortho-carbon (6.33, 1.21)	meta-carbon (6.95, 1.13)	C' (methyl carbon) (4.59, 0.71)		
ethylbenzene	specific C (para-carbon) (5.11, 0.98); (6.99, 0.99); (10.25, 1.24)	substituted carbon (6.57, 1.09)	ortho-carbon (4.47, 0.54)	meta-carbon (4.27, 0.81)	C' (methyl carbon) (4.67, 0.42)	C'' (methylene carbon) (7.53, 0.99)	
o-xylene	specific C (meta-carbon) (4.65, 0.81); (7.07, 1.05); (10.37, 1.22)	substituted carbon (6.53, 1.03)	ortho-carbon (4.59, 0.56)	C' (methyl carbon) (4.71, 0.49)			
p-xylene	specific C (ortho-carbon) (4.25, 0.49); (6.67, 0.92); (10.49, 1.16)	substituted carbon (5.35, 0.90)	C' (methyl carbon) (4.49, 0.72)				
benzene	(4.03, 0.70); (6.67, 1.16); (9.93, 1.30)						
phenol	specific C (substituted carbon) (4.07, 2.26); (6.81, 1.11); (9.65, 1.15)	ortho-carbon (4.05, 1.01)	meta-carbon (5.27, 0.71)	para-carbon (6.27, 1.07)			
1-methylcyclopentene	C1 (5.27, 0.70); (7.97, 0.76)	C2 (4.39, 0.41); (6.75, 0.77)	C3 (4.97,0.57)	C4 (6.87, 7.33)	C5 (4.49, 0.30)	C' (methyl carbon) (4.59, 0.53)	
methyl cyclopentane	substituted-carbon (6.41, 0.59)	ortho-carbon (6.73, 0.60)	meta-carbon (7.27, 0.61)	C' (methyl carbon) (4.17, 0.40)			
methyl cyclohexane	substituted-carbon (5.41, 0.40)	ortho-carbon (4,83, 0.24)	meta-carbon (4.89, 0.31)	para-carbon (4.87, 0.29)	C' (methyl carbon) (4.51, 0.31)		
1-heptene	C1 (4.37, 0.78); (6.93, 0.77)	C2 (5.24, 0.79); (7.30, 0.72)	C3 (6.73, 0.76)	C4 (7.49, 0.75)	C5 (7.91, 0.69)	C6 (5.47, 0.49)	C7 (4.73, 0.40)
n-heptane	C1, C7 (4.31, 0.35)	C2, C6 (5.43, 0.46)	C3, C5 (7.23, 0.52)	C4 (7.69, 0.56)			
ethane	(4.77, 0.19)						
acetylene	(4.17, 0.80); (4.97, 0.86)						
dichloromethane	(3.93, 1.52); (7.21, 1.34); (11.31, 1.25)						

Figure S10 The RDFs for the C(VOC)-S(SO_4^{2-}) interactions in the dry mono VOC-sulfate systems.

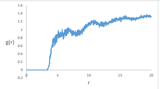
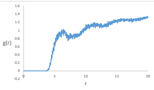
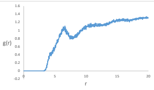
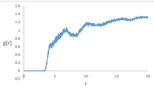
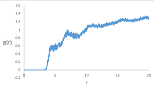
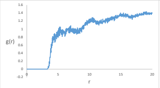
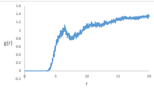
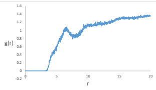
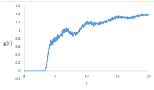
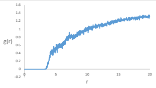
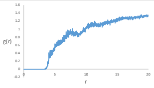
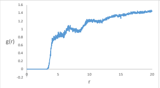
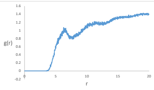
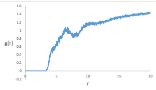
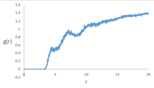
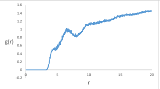
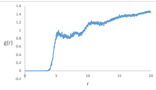
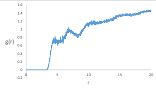
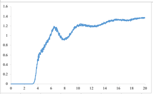
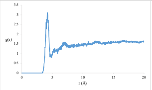
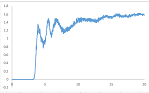
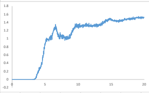
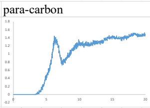
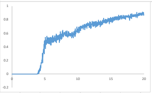
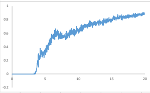
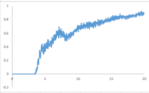
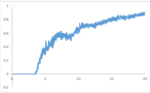
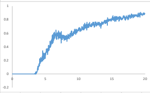
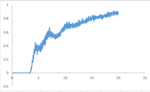
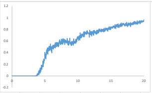
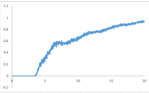
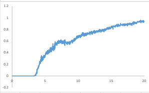
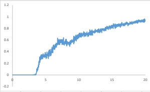
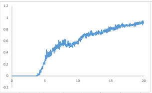
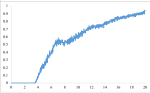
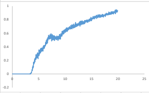
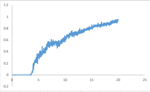
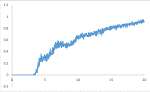
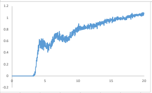
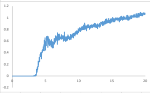
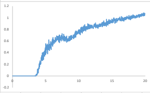
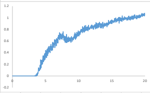
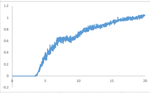
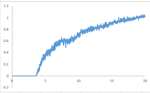
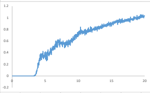
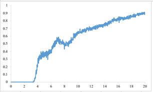
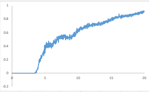
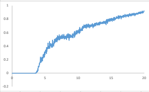
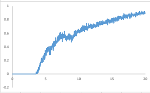
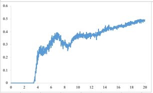
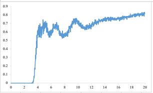
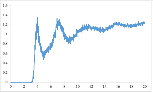
toluene	specific C (para-carbon)  (5.19, 0.81); (6.87, 1.02); (10.73, 1.15)	substituted carbon  (6.11, 0.98)	ortho-carbon  (6.59, 1.10)	meta-carbon  (4.43, 0.61)	C' (methyl carbon)  (4.47, 0.52)		
ethylbenzene	specific C (para-carbon)  (5.15, 1.03); (7.17, 1.00); (10.35, 1.08)	substituted carbon  (6.33, 1.01)	ortho-carbon  (6.55, 1.04)	meta-carbon  (6.63, 1.04)	C' (methyl carbon)  (4.61, 0.51)	C'' (methylene carbon)  (7.73, 0.90)	
o-xylene	specific C (meta-carbon)  (4.69, 0.82); (6.73, 0.99); (10.23, 1.19)	substituted carbon  (6.61, 1.00)	ortho-carbon  (6.69, 1.00)	C' (methyl carbon)  (4.39, 0.49)			
p-xylene	specific C (ortho-carbon)  (4.27,0.47); (6.63,1.00); (10.27, 1.10)	substituted carbon  (5.37, 1.01)	C' (methyl carbon)  4.29, 0.69				
benzene	 (4.21, 0.54); (6.67, 1.13); (10.09, 1.18)						
phenol	specific C (substituted carbon)  (4.23, 2.85); (5.47, 1.18); (7.11, 1.51)	ortho-carbon  (4.09, 1.26)	meta-carbon  (6.57, 1.35)	para-carbon  (6.21, 1.44)			
1-methylcyclopentene	C1  (5.31, 0.47); (8.51, 0.69)	C2  (4.23, 0.38); (6.67, 0.58)	C3  (4.55, 0.37)	C4  (4.61, 0.33)	C5  (4.95, 0.23)	C' (methyl carbon)  (4.37, 0.36)	
methyl cyclopentane	substituted-carbon  (5.67, 0.45)	ortho-carbon  (6.79, 0.53)	meta-carbon  (7.09, 0.58)	C' (methyl carbon)  (4.51, 0.29)			
methyl cyclohexane	substituted-carbon  (5.39, 0.39)	ortho-carbon  (4.87, 0.22)	meta-carbon  (5.05, 0.30)	para-carbon  (5.03, 0.31)	C' (methyl carbon)  (4.51, 0.27)		
1-heptene	C1  (4.59, 0.56); (6.67, 0.69)	C2  (5.11, 0.59); (6.93, 0.67)	C3  (7.13, 0.70)	C4  (7.43, 0.67)	C5  (7.01, 0.63)	C6  (7.19, 0.59)	C7  (4.61, 0.36)
n-heptane	C1, C7  (4.85, 0.34)	C2, C6  (5.45, 0.40)	C3, C5  (7.13, 0.53)	C4  (5.71, 0.39)			
ethane	 (4.41, 0.25)						
acetylene	 (4.67, 0.64); (6.65, 0.65)						
dichloromethane	 (3.81, 1.18); (7.25, 1.22); (11.37, 1.14)						

Figure S11 The RDFs for the C(VOC)-S(SO_4^{2-}) interactions in the aqueous mono VOC-sulfate systems.

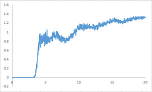
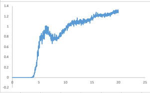
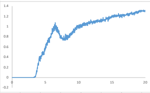
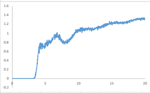
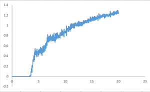
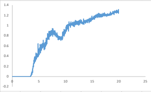
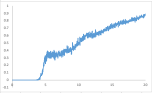
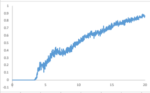
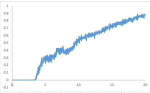
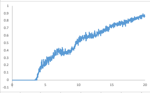
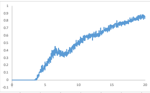
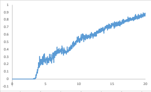
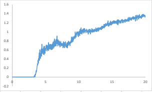
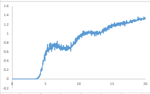
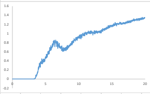
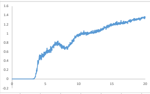
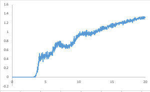
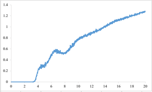
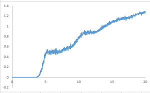
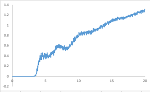
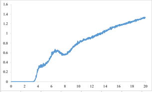
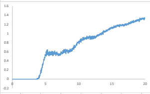
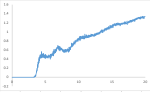
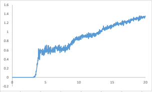
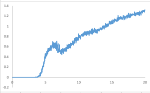
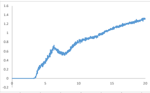
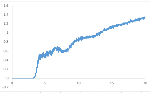
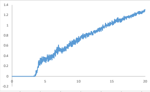
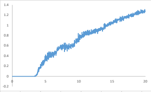
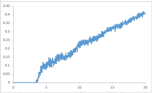
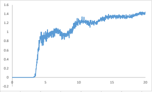
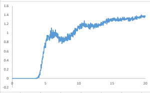
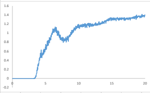
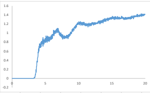
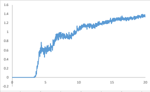
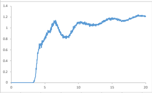
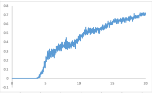
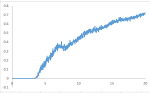
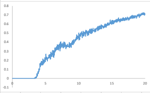
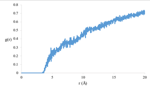
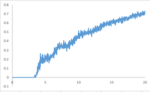
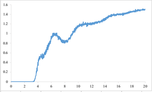
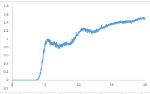
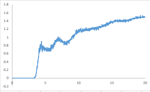
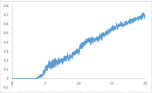
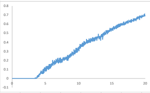
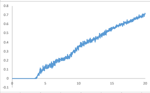
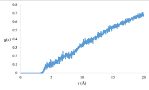
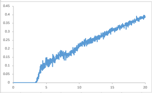
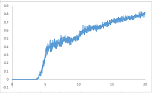
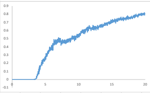
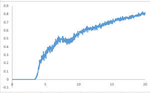
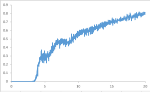
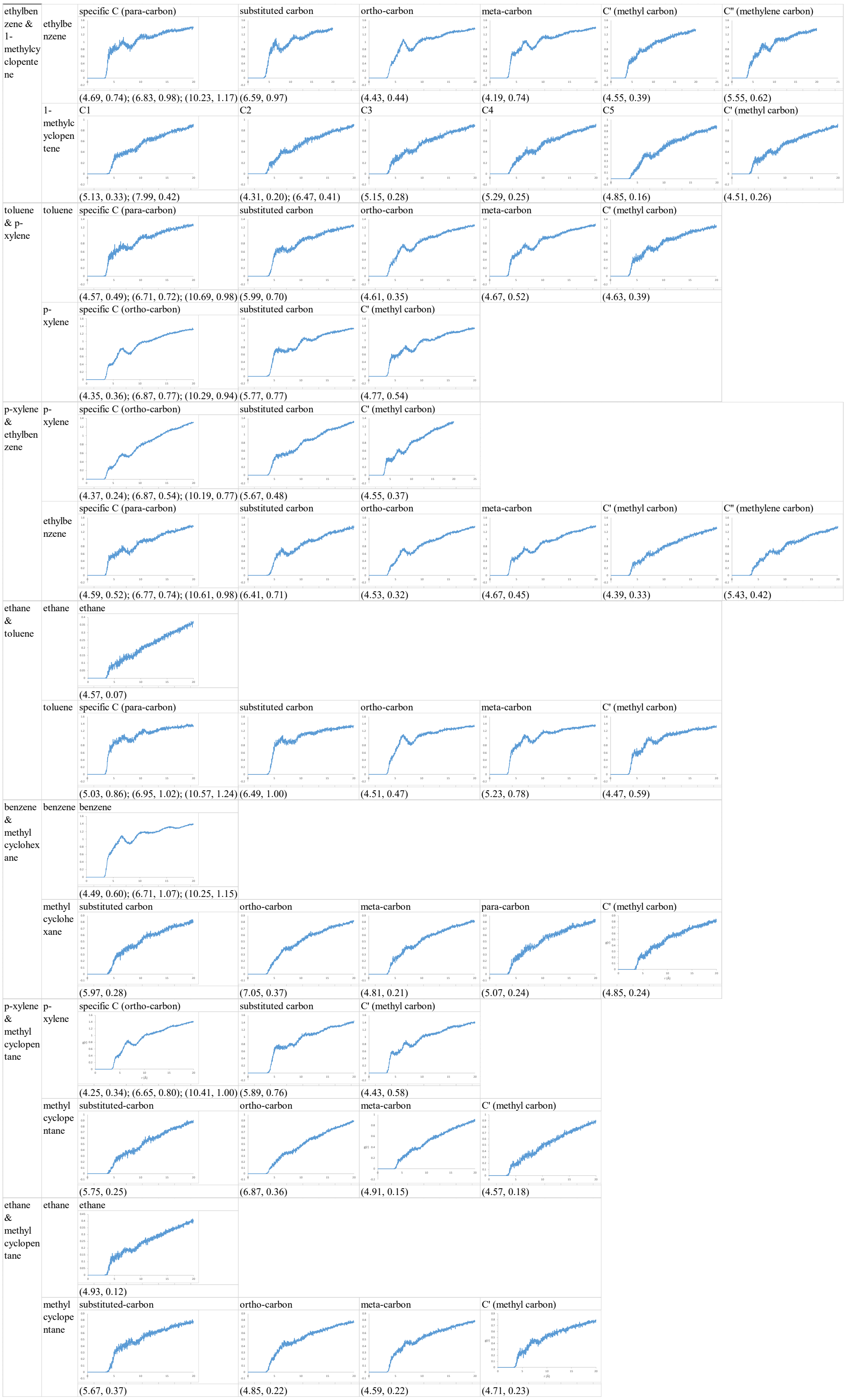
ethylbenzene & 1-methylcyclopentene	ethylbenzene	specific C (para-carbon)  (4.97, 0.89); (6.81, 0.96); (10.29, 1.14)	substituted carbon  (6.43, 0.93)	ortho-carbon  (4.39, 0.42)	meta-carbon  (4.41, 0.76)	C' (methyl carbon)  (4.59, 0.50)	C'' (methylene carbon)  (7.71, 0.88)
	1-methylcyclopentene	C1  (5.27, 0.36); (7.97, 0.42)	C2  (4.31, 0.2); (6.49, 0.41)	C3  (5.13, 0.32)	C4  (4.59, 0.19)	C5  (4.53, 0.15)	C' (methyl carbon)  (4.61, 0.30)
toluene & p-xylene	toluene	specific C (para-carbon)  (4.87, 0.62); (6.89, 0.83); (10.39, 1.04)	substituted carbon  (6.29, 0.77)	ortho-carbon  (4.53, 0.41)	meta-carbon  (4.25, 0.52)	C' (methyl carbon)  (4.91, 0.48)	
	p-xylene	specific C (ortho-carbon)  (4.55, 0.29); (6.69, 0.56); (10.31, 0.80)	substituted carbon  (5.37, 0.51)	C' (methyl carbon)  (4.79, 0.42)			
p-xylene & ethylbenzene	p-xylene	specific C (ortho-carbon)  (4.59, 0.34); (6.71, 0.64); (10.45, 0.82)	substituted carbon  (5.87, 0.57)	C' (methyl carbon)  (4.57, 0.50)			
	ethylbenzene	specific C (para-carbon)  (4.05, 0.60); (6.59, 0.64); (10.63, 0.92)	substituted carbon  (6.35, 0.64)	ortho-carbon  (4.31, 0.28)	meta-carbon  (4.19, 0.50)	C' (methyl carbon)  (4.55, 0.35)	C'' (methylene carbon)  (7.83, 0.66)
ethane & toluene	ethane	ethane  (4.47, 0.11)					
	toluene	specific C (para-carbon)  (4.59, 0.93); (6.41, 1.03); (10.31, 1.26)	substituted carbon  (6.05, 1.02)	ortho-carbon  (4.43, 0.53)	meta-carbon  (4.29, 0.75)	C' (methyl carbon)  (4.57, 0.65)	
benzene & methyl cyclohexane	benzene	benzene  (4.31, 0.71); (6.43, 1.10); (10.23, 1.10)					
	methyl cyclohexane	substituted carbon  (5.53, 0.28)	ortho-carbon  (5.33, 0.22)	meta-carbon  (5.13, 0.23)	para-carbon  (5.07, 0.25)	C' (methyl carbon)  (4.53, 0.21)	
p-xylene & methyl cyclopentane	p-xylene	specific C (ortho-carbon)  (4.59, 0.54); (6.53, 0.99); (10.57, 1.16)	substituted carbon  (5.35, 1.01)	C' (methyl carbon)  (4.49, 0.79)			
	methyl cyclopentane	substituted-carbon  (5.75, 0.18)	ortho-carbon 	meta-carbon 	C' (methyl carbon)  (4.85, 0.11)		
ethane & methyl cyclopentane	ethane	ethane  (4.53, 0.10)					
	methyl cyclopentane	substituted-carbon  (6.17, 0.43)	ortho-carbon  (7.05, 0.49)	meta-carbon  (5.79, 0.38)	C' (methyl carbon)  (4.77, 0.32)		

Figure S12 The RDFs for the C(VOC)-S(SO_4^{2-}) interactions in the dry dual VOCs-sulfate systems.



ethylbenzene & 1-methylcyclopentene	ethylbenzene	specific C (para-carbon)	substituted carbon	ortho-carbon	meta-carbon	C' (methyl carbon)	C" (methylene carbon)
		(4.69, 0.74); (6.83, 0.98); (10.23, 1.17)	(6.59, 0.97)	(4.43, 0.44)	(4.19, 0.74)	(4.55, 0.39)	(5.55, 0.62)
	1-methylcyclopentene	C1	C2	C3	C4	C5	C' (methyl carbon)
		(5.13, 0.33); (7.99, 0.42)	(4.31, 0.20); (6.47, 0.41)	(5.15, 0.28)	(5.29, 0.25)	(4.85, 0.16)	(4.51, 0.26)
toluene & p-xylene	toluene	specific C (para-carbon)	substituted carbon	ortho-carbon	meta-carbon	C' (methyl carbon)	
		(4.57, 0.49); (6.71, 0.72); (10.69, 0.98)	(5.99, 0.70)	(4.61, 0.35)	(4.67, 0.52)	(4.63, 0.39)	
	p-xylene	specific C (ortho-carbon)	substituted carbon	C' (methyl carbon)			
		(4.35, 0.36); (6.87, 0.77); (10.29, 0.94)	(5.77, 0.77)	(4.77, 0.54)			
p-xylene & ethylbenzene	p-xylene	specific C (ortho-carbon)	substituted carbon	C' (methyl carbon)			
		(4.37, 0.24); (6.87, 0.54); (10.19, 0.77)	(5.67, 0.48)	(4.55, 0.37)			
	ethylbenzene	specific C (para-carbon)	substituted carbon	ortho-carbon	meta-carbon	C' (methyl carbon)	C" (methylene carbon)
		(4.59, 0.52); (6.77, 0.74); (10.61, 0.98)	(6.41, 0.71)	(4.53, 0.32)	(4.67, 0.45)	(4.39, 0.33)	(5.43, 0.42)
ethane & toluene	ethane	ethane					
		(4.57, 0.07)					
	toluene	specific C (para-carbon)	substituted carbon	ortho-carbon	meta-carbon	C' (methyl carbon)	
		(5.03, 0.86); (6.95, 1.02); (10.57, 1.24)	(6.49, 1.00)	(4.51, 0.47)	(5.23, 0.78)	(4.47, 0.59)	
benzene & methyl cyclohexane	benzene	benzene					
		(4.49, 0.60); (6.71, 1.07); (10.25, 1.15)					
	methyl cyclohexane	substituted carbon	ortho-carbon	meta-carbon	para-carbon	C' (methyl carbon)	
		(5.97, 0.28)	(7.05, 0.37)	(4.81, 0.21)	(5.07, 0.24)	(4.85, 0.24)	
p-xylene & methyl cyclopentane	p-xylene	specific C (ortho-carbon)	substituted carbon	C' (methyl carbon)			
		(4.25, 0.34); (6.65, 0.80); (10.41, 1.00)	(5.89, 0.76)	(4.43, 0.58)			
	methyl cyclopentane	substituted-carbon	ortho-carbon	meta-carbon	C' (methyl carbon)		
		(5.75, 0.25)	(6.87, 0.36)	(4.91, 0.15)	(4.57, 0.18)		
ethane & methyl cyclopentane	ethane	ethane					
		(4.93, 0.12)					
	methyl cyclopentane	substituted-carbon	ortho-carbon	meta-carbon	C' (methyl carbon)		
		(5.67, 0.37)	(4.85, 0.22)	(4.59, 0.22)	(4.71, 0.23)		

Figure S13 The RDFs for the C(VOC)-S(SO_4^{2-}) interactions in the aqueous dual VOCs-sulfate systems.

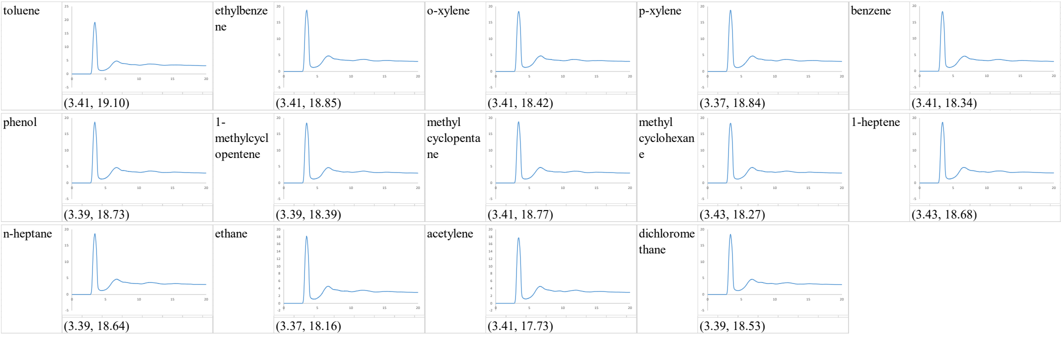


Figure S14 The RDFs for the S(SO_4^{2-})-O(H_3O^+) interactions in the aqueous mono VOC-sulfate systems.

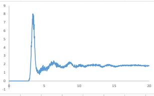
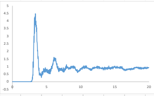
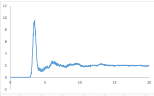
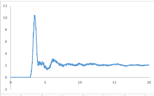
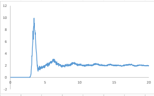
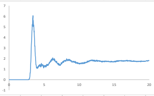
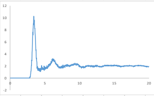
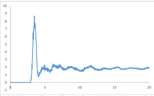
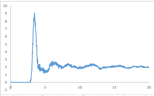
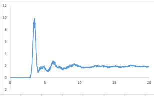
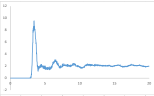
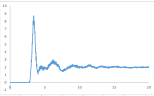
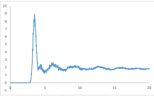
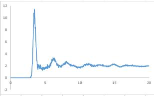
toluene	 (3.51, 7.28)	ethylbenzene	 (3.37, 4.48)	o-xylene	 (3.49, 9.52)	p-xylene	 (3.43, 10.43)	benzene	 (3.41, 9.95)
phenol	 (3.39, 6.05)	1-methylcyclopentene	 (3.39, 10.26)	methyl cyclopentane	 (3.43, 8.70)	methyl cyclohexane	 (3.45, 9.06)	1-heptene	 (3.53, 9.89)
n-heptane	 (3.41, 9.53)	ethane	 (3.39, 8.74)	acetylene	 (3.47, 8.93)	dichloromethane	 (3.43, 11.40)		

Figure S15 The RDFs for the S(SO_4^{2-})-O(H_2O) interactions in the aqueous mono VOC-sulfate systems.

toluene	C1 (substituted carbon) (4.99, 9.98)	C2 (ortho-carbon) (3.97, 7.14)	C3 (meta-carbon) (3.91, 10.28)	C4 (para-carbon) (3.81, 12.30)	C' (substituent carbon) (4.21, 8.76)		
ethylbenzene	C1 (substituted carbon) (5.51, 5.14)	C2 (ortho-carbon) (3.85, 3.55)	C3 (meta-carbon) (3.97, 4.83)	C4 (para-carbon) (3.63, 5.63)	C' (methyl carbon) (4.11, 4.16)	C'' (methylene carbon) (4.63, 4.55)	
o-xylene	C1 (substituted carbon) (5.13, 10.19)	C2 (ortho-carbon) (3.89, 10.60)	C3 (meta-carbon) (3.75, 14.61)	C' (substituent carbon) (3.99, 9.10)			
p-xylene	C1 (substituted carbon) (4.91, 9.30)	C2 (ortho-carbon) (4.17, 6.05)	C' (substituent carbon) (4.19, 8.74)				
benzene	(4.19, 7.59)						
phenol	C1 (substituted carbon) (1.37, 2598.87)	C2 (ortho-carbon) (2.41, 498.44)	C3 (meta-carbon) (3.67, 230.39)	C4 (para-carbon) (4.17, 171.38)			
1-methylcyclopentene	C1 (4.81, 5.31)	C2 (3.69, 4.23)	C3 (4.27, 4.63)	C4 (5.13, 4.52)	C5 (5.97, 4.63)	C' (substituent carbon) (3.97, 5.60)	
methyl cyclopentane	C1 (substituted carbon) (5.03, 2.27)	C2 (ortho-carbon) (5.91, 1.98)	C3 (meta-carbon) (5.73, 1.99)	C' (substituent carbon) (4.27, 2.10)			
methyl cyclohexane	C1 (substituted carbon) (5.01, 6.64)	C2 (ortho-carbon) (6.13, 5.52)	C3 (meta-carbon) (4.55, 4.96)	C4 (para-carbon) (4.73, 5.72)	C' (substituent carbon) (3.69, 5.41)		
1-heptene	C1 (3.83, 8.26)	C2 (4.53, 6.86)	C3 (5.31, 6.10)	C4 (5.77, 5.99)	C5 (5.89, 5.52)	C6 (4.93, 6.11)	C7 (4.15, 6.36)
n-heptane	C1 (C7) (4.09, 3.96)	C2 (C6) (4.95, 4.06)	C3 (C5) (5.19, 4.05)	C4 (5.81, 4.04)			
ethane	(4.47, 1.21)						
acetylene	(3.87, 4.23)						
dichloromethane	(3.51, 13.43)						

Figure S16 The RDFs for the C(VOC)-O(H_2O) interactions in the aqueous mono VOC-sulfate systems.

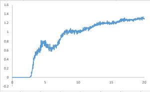
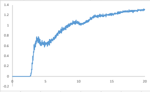
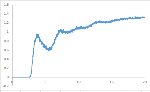
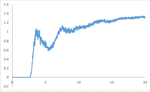
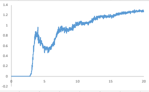
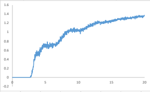
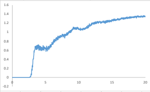
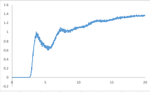
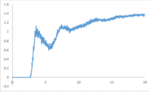
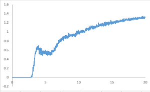
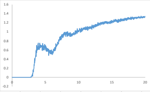
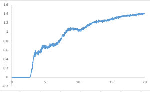
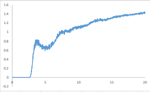
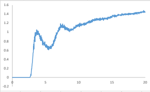
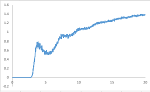
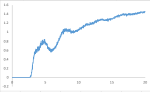
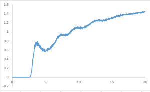
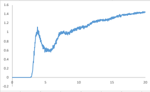
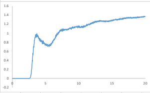
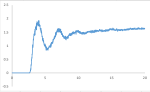
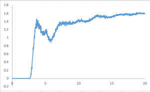
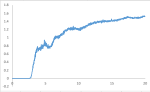
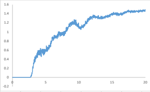
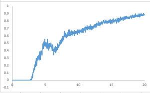
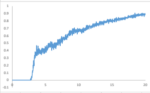
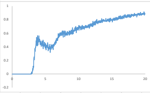
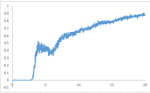
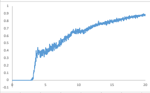
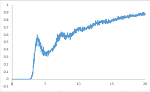
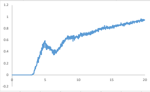
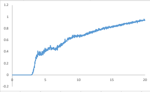
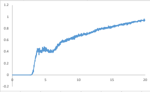
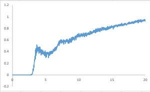
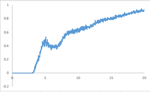
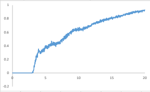
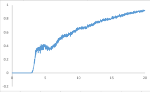
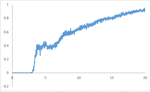
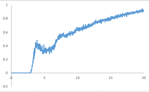
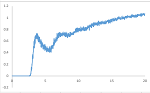
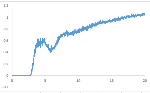
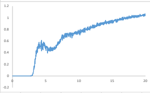
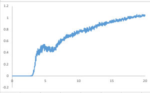
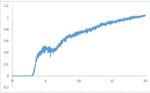
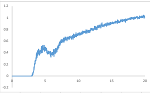
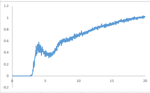
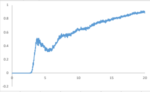
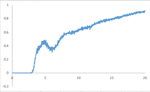
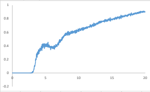
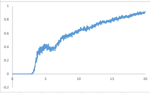
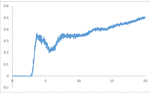
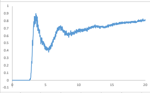
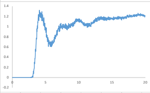
toluene	C1 (substituted carbon)  (4.77, 0.79)	C2 (ortho-carbon)  (3.83, 0.74)	C3 (meta-carbon)  (3.91, 0.92)	C4 (para-carbon)  (3.73, 0.98)	C' (substituent carbon)  (3.83, 0.83)		
ethylbenzene	C1 (substituted carbon)  (4.79, 0.70)	C2 (ortho-carbon)  (4.09, 0.70)	C3 (meta-carbon)  (3.71, 0.94)	C4 (para-carbon)  (3.73, 1.05)	C' (methyl carbon)  (3.95, 0.64)	C'' (methylene carbon)  (4.31, 0.71)	
o-xylene	C1 (substituted carbon)  (3.71, 0.54)	C2 (ortho-carbon)  (3.83, 0.80)	C3 (meta-carbon)  (3.79, 1.03)	C' (substituent carbon)  (3.89, 0.76)			
p-xylene	C1 (substituted carbon)  (4.71, 0.79)	C2 (ortho-carbon)  (3.69, 0.72)	C' (substituent carbon)  (3.77, 1.04)				
benzene	 (3.77, 0.94)						
phenol	C1 (substituted carbon)  (3.77, 1.89)	C2 (ortho-carbon)  (3.87, 1.34)	C3 (meta-carbon)  (4.17, 0.76)	C4 (para-carbon)  (4.45, 0.59)			
1-methylcyclopentene	C1  (4.87, 0.50)	C2  (3.91, 0.41)	C3  (3.93, 0.50)	C4  (4.21, 0.47)	C5  (3.91, 0.40)	C' (substituent carbon)  (3.87, 0.56)	
methyl cyclopentane	C1 (substituted carbon)  (4.93, 0.56)	C2 (ortho-carbon)  (4.03, 0.40)	C3 (meta-carbon)  (4.61, 0.46)	C' (substituent carbon)  (3.79, 0.46)			
methyl cyclohexane	C1 (substituted carbon)  (5.05, 0.47)	C2 (ortho-carbon)  (4.07, 0.33)	C3 (meta-carbon)  (4.47, 0.37)	C4 (para-carbon)  (4.63, 0.41)	C' (substituent carbon)  (3.85, 0.42)		
1-heptene	C1  (3.81, 0.69)	C2  (4.11, 0.58)	C3  (4.35, 0.56)	C4  (4.83, 0.51)	C5  (4.99, 0.47)	C6  (4.75, 0.48)	C7  (4.19, 0.51)
n-heptane	C1 (C7)  (3.87, 0.49)	C2 (C6)  (4.73, 0.46)	C3 (C5)  (5.01, 0.42)	C4  (5.13, 0.43)			
ethane	 (3.77, 0.35)						
acetylene	 (3.51, 0.87)						
dichloromethane	 (4.23, 1.27)						

Figure S17 The RDFs for the C(VOC)-O(H_3O^+) interactions in the aqueous mono VOC-sulfate systems.