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Supplementary Information Debye screening, over-screening and specific adsorption in solutions of organic ions †

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Table 1 Force field parameters for the DCE molecule. Refer to Figure 1 in the main paper for definitions of atom types.

Atom type	σ (nm)	ε(kj/mol)	q (e)
Cl	0.34	1.2552	-0.27
CH_2	0.38	0.493712	0.27

Table 2 Intramolecular interactions between atoms in the DCE molecule. r_b is the bond length between pairs of atoms. θ_0 and k_θ the equilibrium angle and the force constant of the three body angle potential, $U(\theta_{ijk}) = k_\theta/2(\theta-\theta_0)^2$. The dihedral angle is defined as, $U(\phi_{ijkl}) = k_\phi(1+cos(n\phi-\phi_0))$. Refer to Figure 1 in the main paper for definitions of atom types.

Atoms	r_b (nm)		
Cl-CH_2	0.178		
CH_2-CH_2	0.153		
Atoms	k_θ (kj/(mol rad^2))	θ_0 (deg)	
Cl-CH_2-CH_2	520	108.2	
Atoms	k_ϕ (kj/(mol rad^2))	n	ϕ_0 (deg)
Cl-CH_2-CH_2-Cl	5.9	3	0

Table 3 Force field parameters for the TBA cation: σ in nm, ε in kj/mol, charge in e. Refer to Figure 1 in the main paper for definitions of atom types.

Atom type	σ	ε	q
C44, C34, C24, C14	3.74792e-01	8.67150e-01	0.041
C43, C33, C23, C13	4.07038e-01	4.10542e-01	0.033
C12, C22, C32, C42	4.07038e-01	4.10542e-01	0.020
C41, C11, C31, C21	4.07038e-01	4.10542e-01	0.015
N1	3.13647e-01	6.39795e-01	0.564

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Table 4 Intramolecular interactions for TBA cation. r_b represents the bond length between pairs of atoms. θ_0 k_θ the equilibrium angle and the force constant of the three body angle potential, $U(\theta_{ijk}) = k_\theta/2(\theta - \theta_0)^2$. The dihedral angle is defined by the potential, $U(\phi_{ijkl}) = k_\phi(1 + cos(n\phi - \phi_0))$. Refer to Figure 1 in the main paper for definitions of atom types.

Atoms	r_b (nm)		
N1-C11, N1-C31, N1-C21, N1-C41	0.1530		
C31-C32, C21-C22, C11-C12, C42-C41	0.1530		
C12-C13, C32-C33, C33-C34	0.1520		
C22-C23, C23-C24, C13-C14	0.1520		
C44-C43, C43-C42	0.1540		
Atoms	k_θ (kj/(mol rad^2))	θ_0 (deg)	
C44-C43-C42, C43-C42-C41, C42-C41-N1	111.00	530.00	
N1-C11-C12, C11-C12-C13, N1-C31-C32	111.00	530.00	
C31-C32-C33, C32-C33-C34, N1-C21-C22	111.00	530.00	
C21-C22-C23, C22-C23-C24, C12-C13-C14	111.00	530.00	
C41-N1-C11, C41-N1-C31, C41-N1-C21	109.00	1680.51	
C11-N1-C31, C11-N1-C21, C31-N1-C21	109.00	1680.51	
Atoms	k_ϕ (kj/(mol rad^2))	n	ϕ_0 (deg)
C44-C43-C42-C41, C43-C42-C41-N1, N1-C11-C12-C13	5.92	3	0
C11-C12-C13-C14 , N1-C31-C32-C33, C31-C32-C33-C34	5.92	3	0
N1-C21-C22-C23, C21-C22-C23-C24	5.92	3	0
C42-C41-N1-C11, C21-N1-C11-C12	1.05	3	0
C11-N1-C31-C32, C11-N1-C21-C22	1.05	3	0

Table 5 Force field parameters for TPB anion: σ in nm, ε in kj/mol, charge in e. Refer to Figure 1 in the main paper for definitions of atom types.

Atom type	σ	ε	q
C1, C4, C11, C15	5.01918e-01	9.48893e-02	-0.047
C19, C9, C23, C22	5.01918e-01	9.48893e-02	-0.047
C25, C16, C18, C8	5.01918e-01	9.48893e-02	-0.034
C5, C20, C12, C6	5.01918e-01	9.48893e-02	-0.034
C21, C3, C10, C14	3.58118e-01	2.77406e-01	0.565
C17, C7, C13, C24	5.01918e-01	9.48893e-02	0.007
B1	3.58118e-01	2.774057e-01	-2.640

Table 6 Intramolecular interactions for the TPB anion. r_b represents the bond length between pairs of atoms. θ_0 k_θ the equilibrium angle and the force constant of the three body angle potential, $U(\theta_{ijk}) = k_\theta/2(\theta - \theta_0)^2$. The dihedral angle is defined by the potential, $U(\phi_{ijkl}) = k_\phi(1 + cos(n\phi - \phi_0))$. Improper dihedrals, $U(\xi_{ijkl}) = k_\xi/2(1 + cos(\xi_{ijkl} - \xi_0))$. Refer to Figure 1 in the main paper for definitions of atom types.

Atoms	r_b (nm)		
C1-C25, C25-C24, C4-C5, C11-C12	0.1390		
C15-C16, C16-C17, C19-C18, C18-C17	0.1390		
C9-C8, C8-C7, C7-C5, C23-C20	0.1390		
C20-C13, C13-C12, C22-C6, C6-C24	0.1390		
C1-C21, C21-C22, C3-C4, C3-C9	0.14		
C10-C11, C10-C23, C14-C15, C14-C19	0.14		
C21-B1, B1-C3, B1-C10, B1-C14	0.1560		
Atoms	k_θ (kj/(mol rad^2))	θ_0 (deg)	
C25-C1-C21, C1-C25-C24, C1-C21-B1	560	120	
C1-C21-C22, B1-C21-C22	560	120	
C21-B1-C3, C21-B1-C10, C21-B1-C14, C3-B1-C10	540	111	
C3-B1-C14, C10-B1-C14	560	120	
B1-C3-C4, B1-C3-C9, C4-C3-C9, C3-C4-C5	560	120	
B1-C10-C11, B1-C10-C23, C11-C10-C23, C10-C11-C12	560	120	
B1-C14-C15, B1-C14-C19, C15-C14-C19, C14-C15-C16	560	120	
C15-C16-C17, C14-C19-C18, C19-C18-C17, C16-C17-C18	560	120	
C3-C9-C8, C9-C8-C7, C8-C7-C5, C4-C5-C7	560	120	
C10-C23-C20, C23-C20-C13, C20-C13-C12, C11-C12-C13	560	120	
C21-C22-C6, C22-C6-C24, C25-C24-C6	560	120	
Atoms	k_ξ (kj/(mol rad^2))		ξ_0 (deg)
C3-B1-C4-C9	167.36		0
C10-B1-C11-C23	167.36		0
C14-B1-C15-C19	167.36		0
C21-C1-B1-C22	167.36		0
Atoms	k_ϕ (kj/(mol rad^2))	n	ϕ_0 (deg)
C21-C1-C25-C24, C25-C1-C21-C22, C1-C25-C24-C6	41.80	2	180
C1-C21-B1-C3, C3-B1-C10-C11	1	6	180
C10-B1-C3-C4, C3-B1-C14-C15	1	6	0
C1-C21-C22-C6, C9-C3-C4-C5, C4-C3-C9-C8, C3-C4-C5-C7	41.80	2	180
C23-C10-C11-C12, C11-C10-C23-C20	41.80	2	180
C10-C11-C12-C13, C19-C14-C15-C16	41.80	2	180
C15-C14-C19-C18, C14-C15-C16-C17	41.80	2	180
C15-C16-C17-C18, C14-C19-C18-C17	41.80	2	180
C19-C18-C17-C16, C3-C9-C8-C7	41.80	2	180
C9-C8-C7-C5, C8-C7-C5-C4	41.80	2	180
C10-C23-C20-C13, C23-C20-C13-C12, C20-C13-C12-C11	41.80	2	180
C21-C22-C6-C24, C22-C6-C24-C25	41.80	2	180