Supporting Information:

Understanding Three Hydration-dependent Transitions of Zwitterionic Carboxybetaine Hydrogel by Molecular Dynamics Simulations

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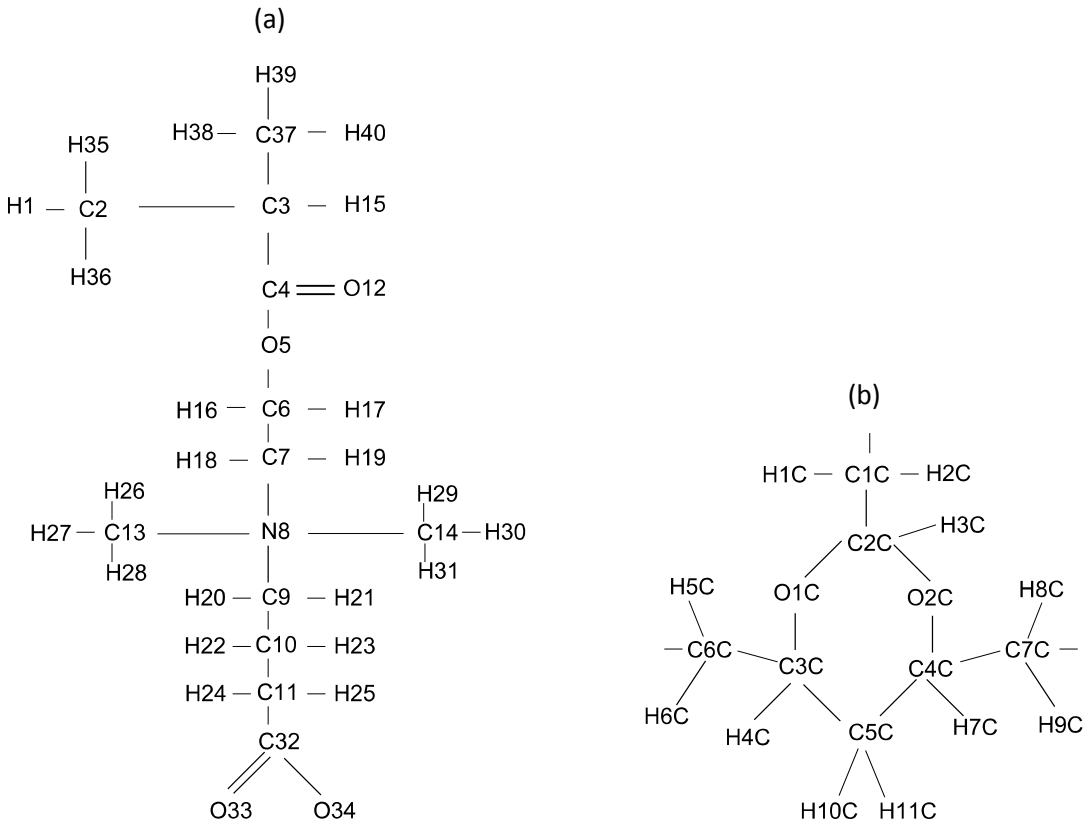

Figure S1. The structure of (a) a CBMA monomer and (b) a 1,3-dioxane cyclic junction.

Table S1. Partial charges of atoms in a CBMA monomer. The atoms are defined in Figure S1(a).

Atom	Partial charge
C2	-0.504
H1, H35, H36	0.138
C37	-0.357
H38, H39, H40	0.101
C3	0.136
H15	0.036
C4	0.808
O12	-0.582
O5	-0.484
C6	0.196
H16, H17	0.064
C7	-0.150
H18, H19	0.122
C13, C14	-0.404
H26, H27, H28, H29, H30, H31	0.193
N8	0.136
C9	-0.265
H20, H21	0.148
C10	0.225
H22, H23	-0.016
C11	-0.356
H24, H25	0.075
C32	0.924
O33, O34	-0.808

Table S2. Partial charges of atoms in a 1,3-dioxane cyclic junction. The atoms are defined in Figure S1(b).

Atom	Partial charge
C1C	-0.200
H1C, H2C	0.100
C2C	0.200
H3C	0.100
O1C, O2C	-0.300
C3C, C4C	0.050
C5C	-0.200
H4C, H7C	0.100
C6C, C7C	-0.200
H5C, H6C, H8C, H9C	0.100
H10C, H11C	0.100