Supplementary Information: Thermodynamic properties of water in aqueous amine solutions studied by energy-representation method

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Contents

1. Computational details

Table S1 Number of molecules of each component in the solution

	Before CO_2 absorption/carbamate		Bicarbonate(all)		Bicarbonate(half)	
EAE [wt%]	water	others	water	others	water	others
0	3333	0	3333	0	3333	0
9.27	2984	62	2922	124	2953	93
18.7	2640	122	2518	244	2579	183
28.3	2300	182	2118	364	2209	273
38	1962	242	1720	484	1841	363
47.9	1622	302	1320	604	1471	453
58	1292	360	932	720	1112	540
68.2	964	418	546	836	755	627
78.6	636	476	160	952	398	714
83.2	-	-	0	846	-	-
89.2	318	532	-	-	52	798
90.8	-	-	-	-	0	750
100	0	588	-	-	-	-

2. Water vapor pressure

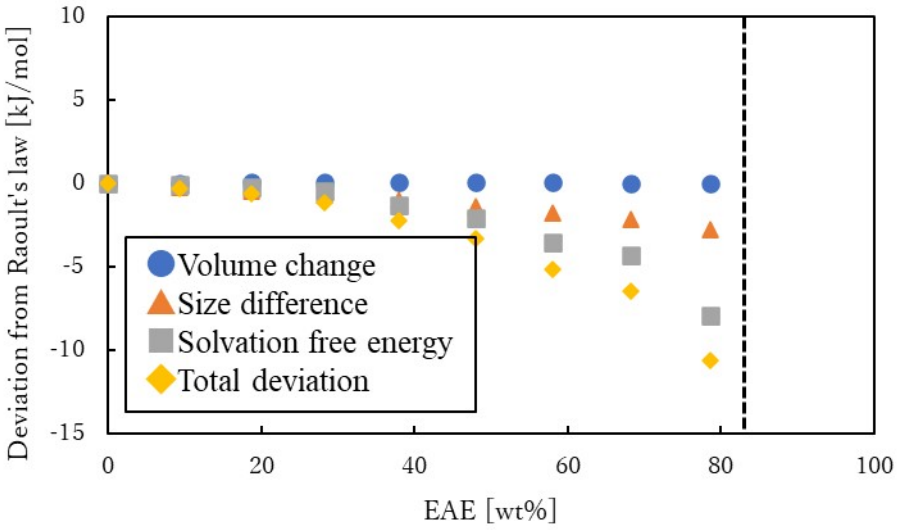

Figure S1 Deviations from Raoult's law and contributions from volume change, size difference, and solvation free energy after bicarbonate-type reaction (all). The vertical dashed line in the graph indicates the EAE concentration at which water is completely consumed by the reaction.

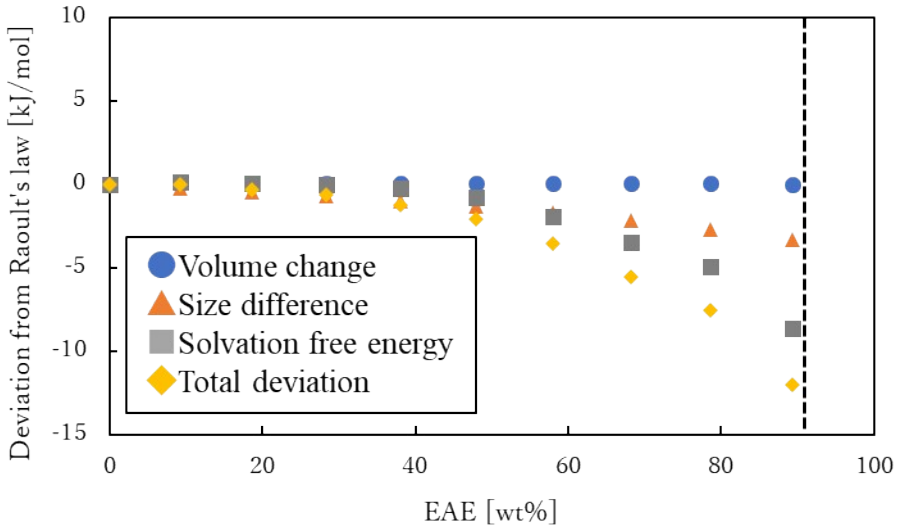

Figure S2 Deviations from Raoult's law and contributions from volume change, size difference, and solvation free energy after bicarbonate-type reaction (half). The vertical dashed line in the graph indicates the EAE concentration at which water is completely consumed by the reaction.

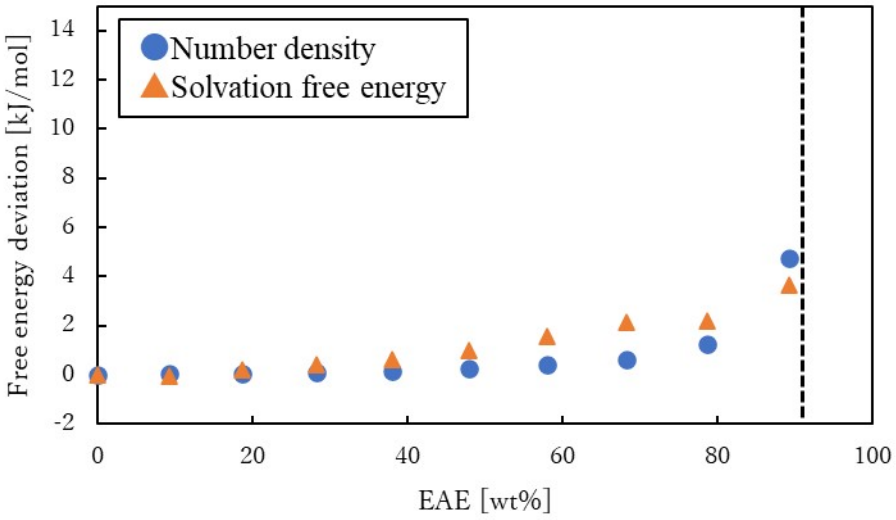

Figure S3 Contribution of water number density and solvation free energy to the difference in water vapor pressure between the carbamate-type and bicarbonate-type reaction (half). The vertical dashed line in the graph indicates the EAE concentration at which water is completely consumed by the reaction.

3. Interaction between water and solvent molecules

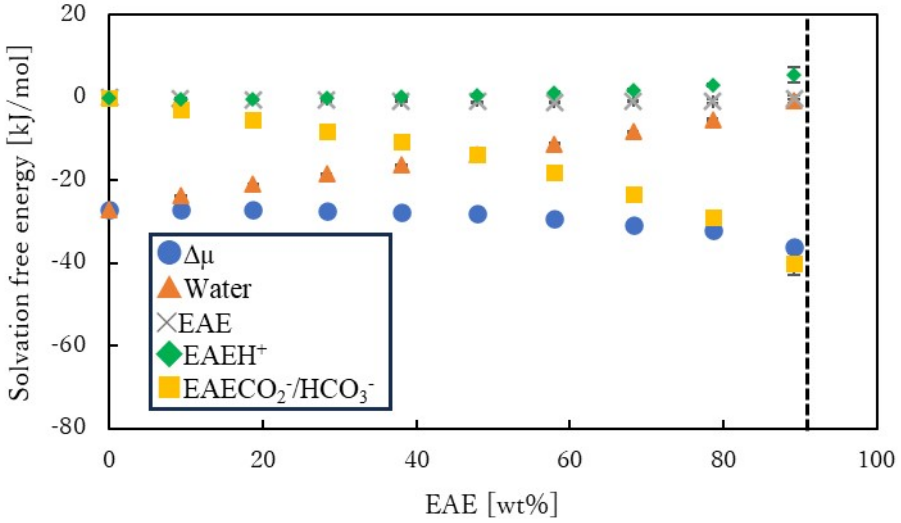

Figure S4 Solvation free energy of water(Δμ) and contribution of each component after bicarbonate-type reaction (half). The vertical dashed line in the graph indicates the EAE concentration at which water is completely consumed by the reaction.

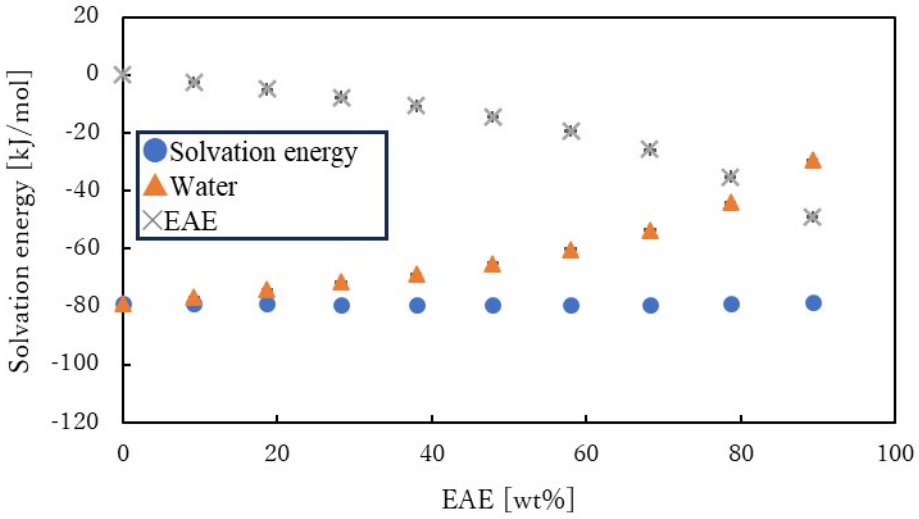

Figure S5 Solvation energy of water and contribution of each component before CO_2 absorption

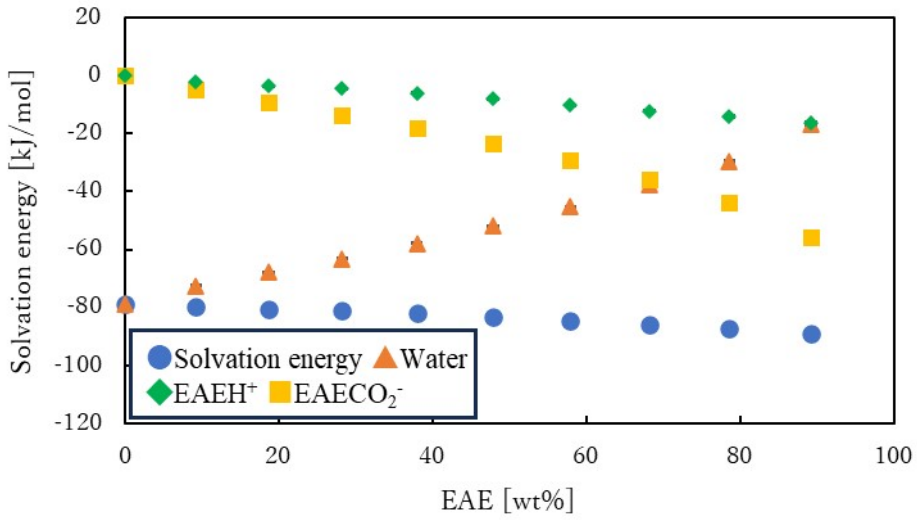

Figure S6 Solvation energy of water and contribution of each component after carbamate-type reaction

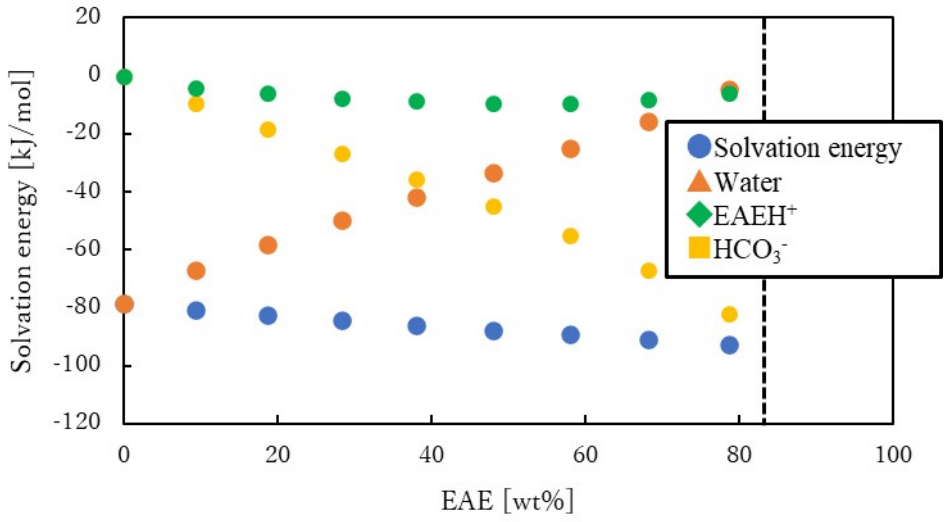

Figure S7 Solvation energy of water and contribution of each component after bicarbonate-type reaction (all). The vertical dashed line in the graph indicates the EAE concentration at which water is completely consumed by the reaction.

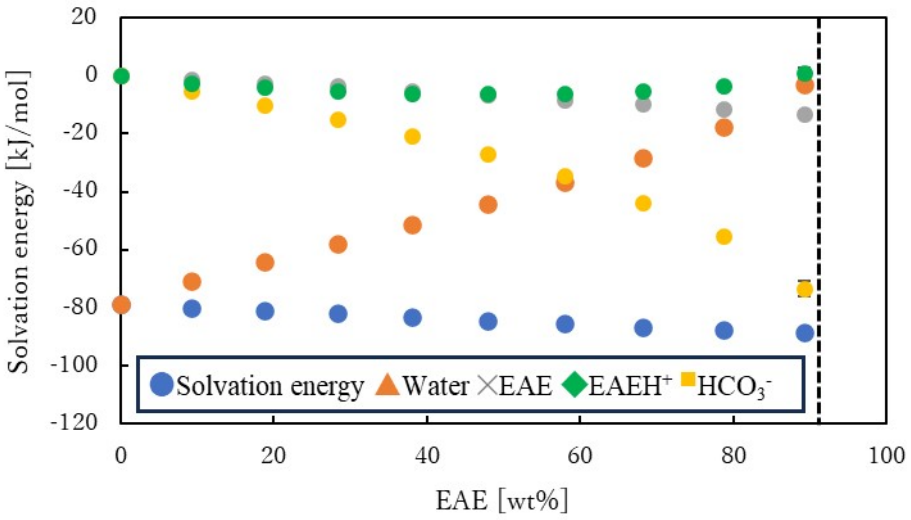

Figure S8 Solvation energy of water and contribution of each component after bicarbonate-type reaction (half). The vertical dashed line in the graph indicates the EAE concentration at which water is completely consumed by the reaction.

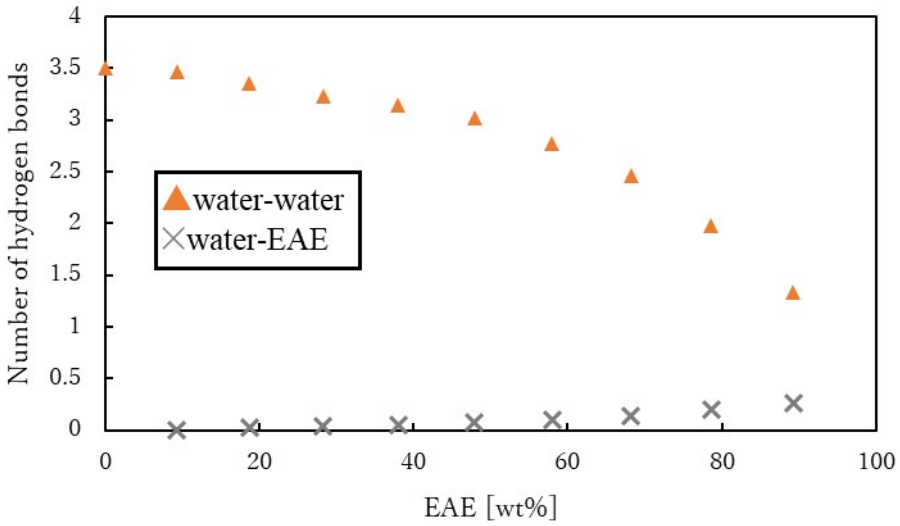

Figure S9 Number of hydrogen bonds before CO_2 absorption

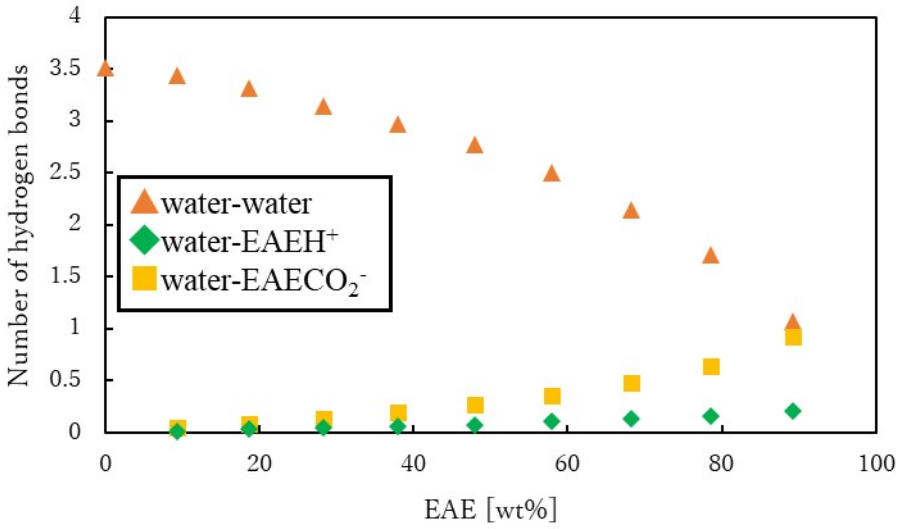

Figure S10 Number of hydrogen bonds after carbamate-type reaction

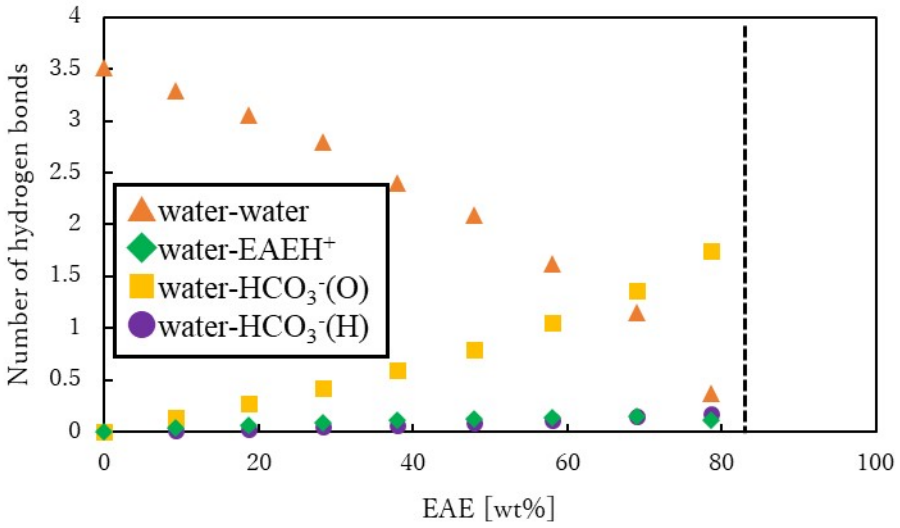

Figure S11 Number of hydrogen bonds after bicarbonate-type reaction (all). The vertical dashed line in the graph indicates the EAE concentration at which water is completely consumed by the reaction.

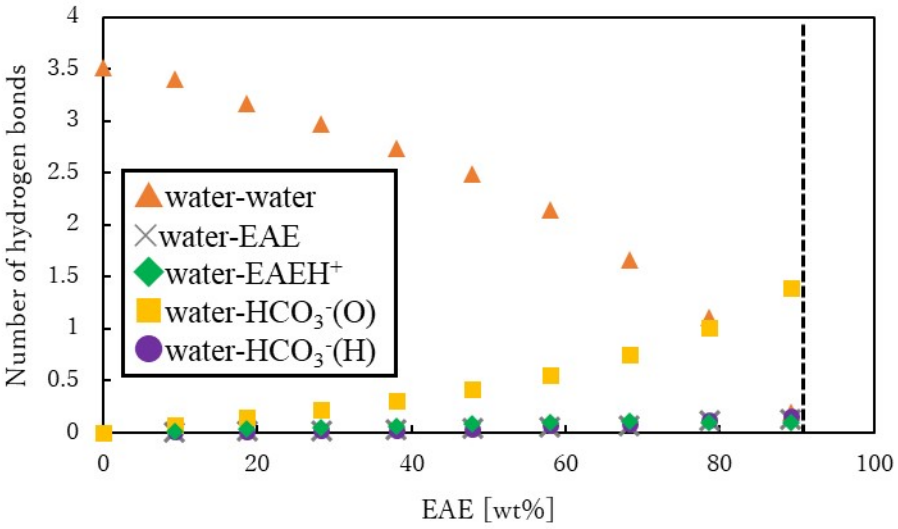

Figure S12 Number of hydrogen bonds after bicarbonate-type reaction (half). The vertical dashed line in the graph indicates the EAE concentration at which water is completely consumed by the reaction.

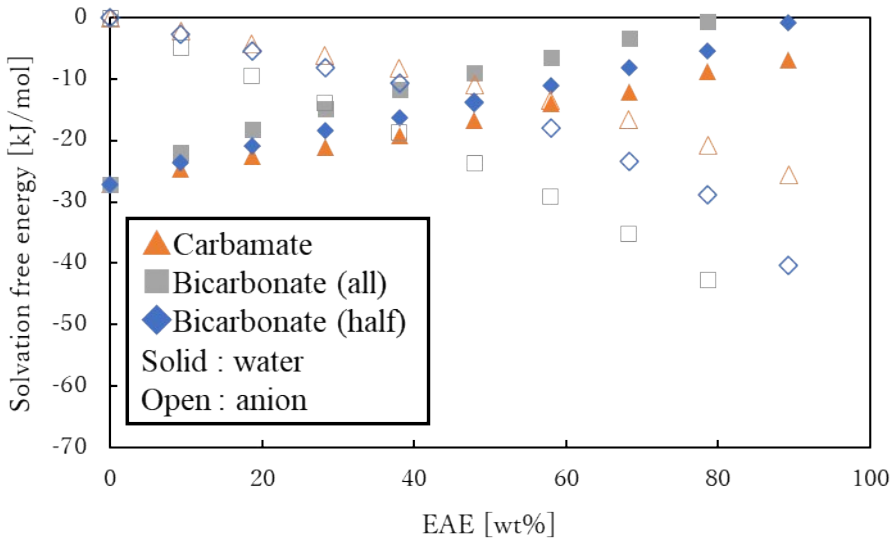

Figure S13 Contributions of water and anions to the solvation free energy

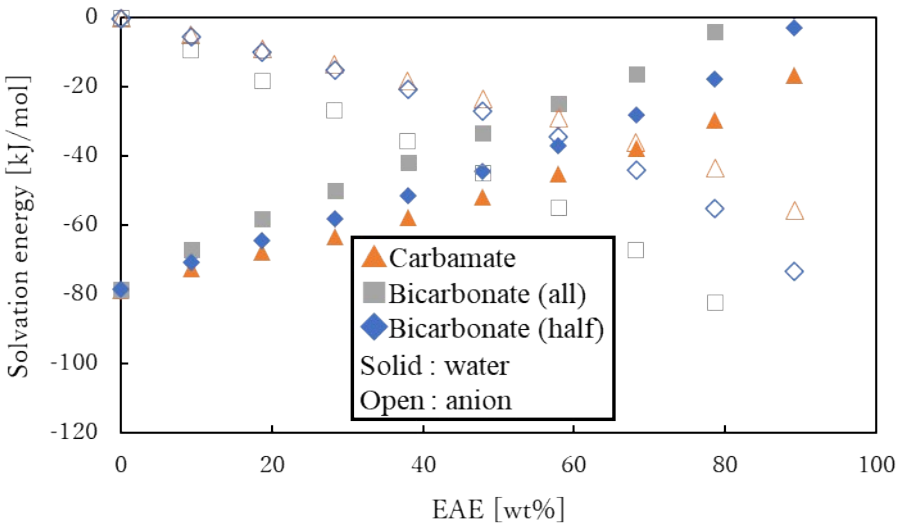

Figure S14 Contributions of water and anions to the solvation energy

4. Temperature dependence of vapor pressure and enthalpy of vaporization

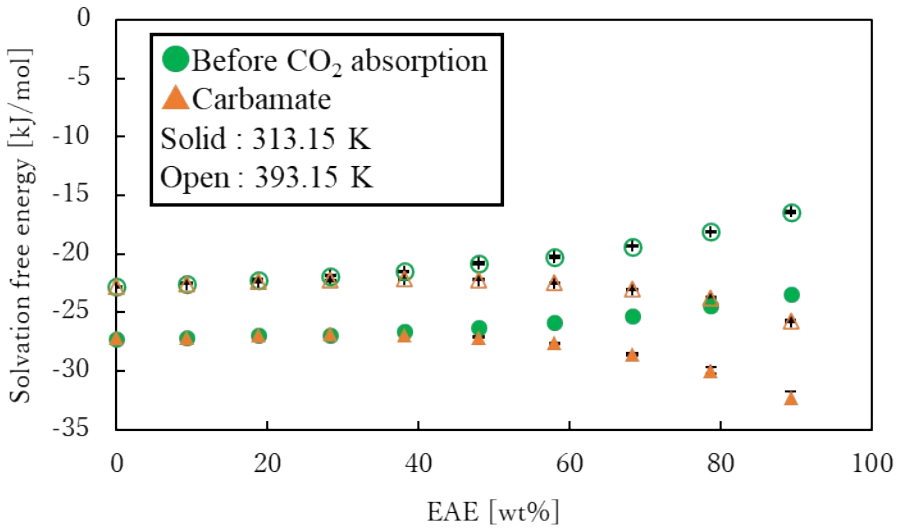

Figure S15 Temperature dependence of solvation free energy

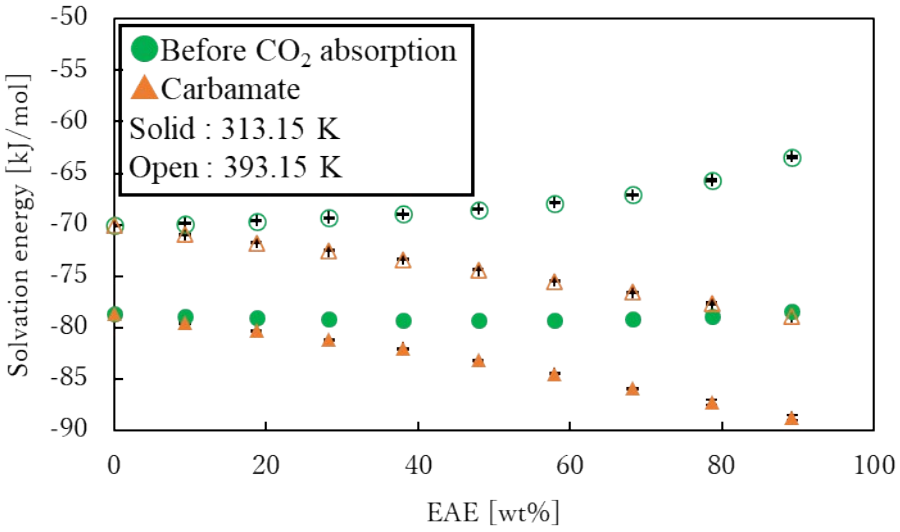

Figure S16 Temperature dependence of solvation energy

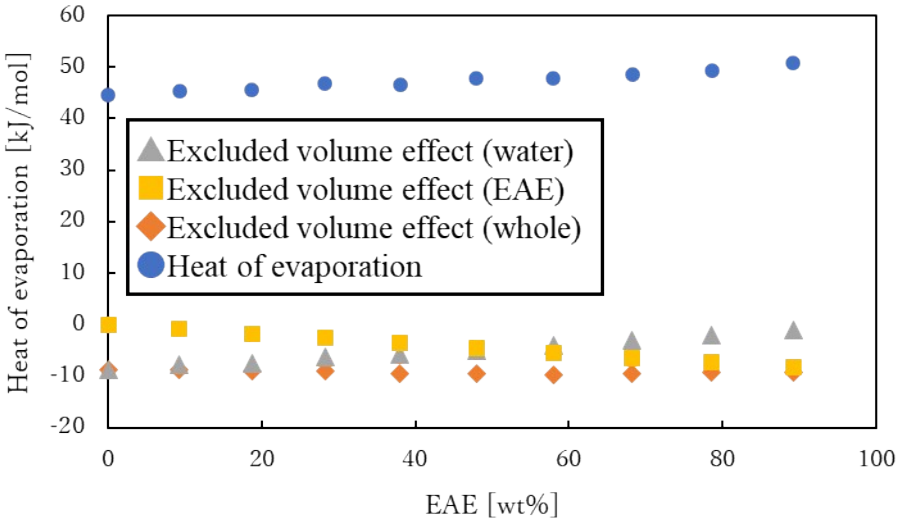

Figure S17 Excluded volume effect to the heat of evaporation

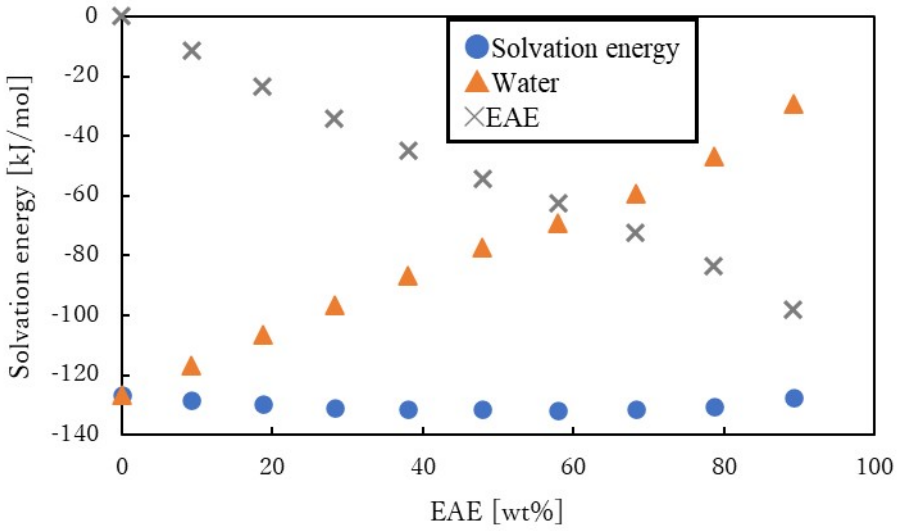

Figure S18 Solvation energy of EAE and contribution of each component before CO_2 absorption

5. Concentration fluctuation of water and vapor pressure

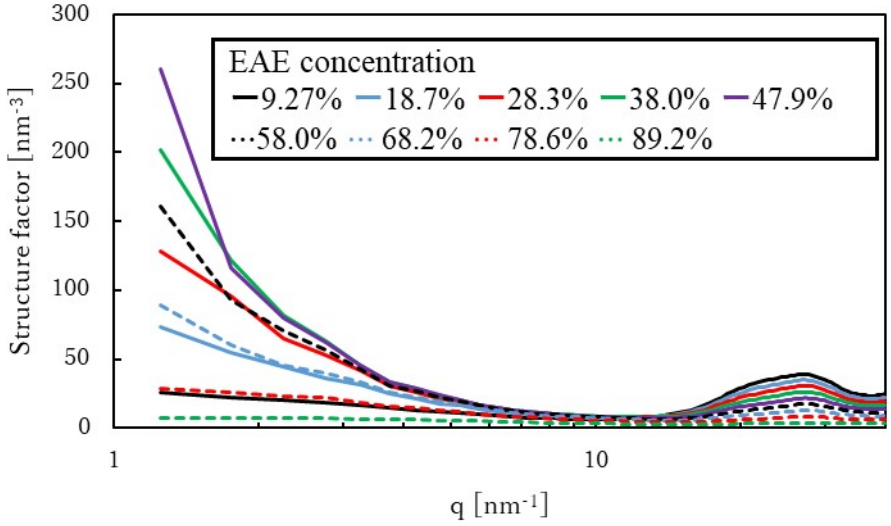

Figure S19 Structure factor before CO_2 absorption

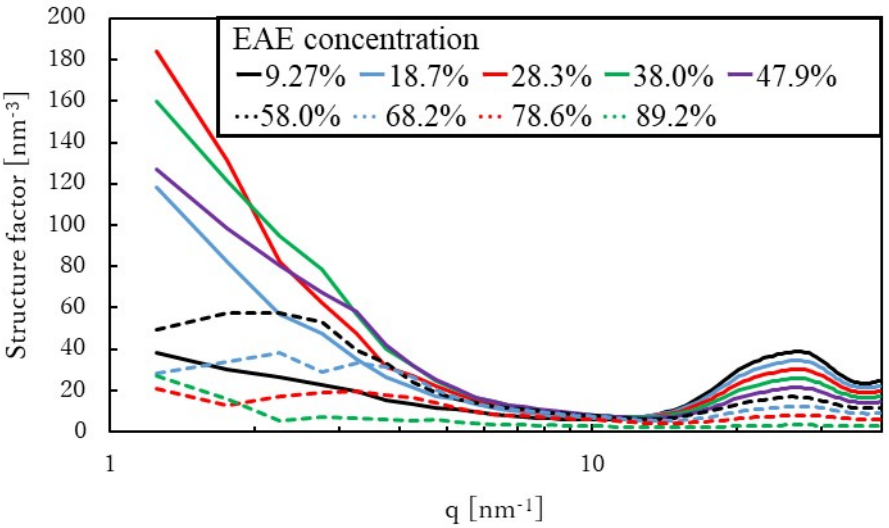

Figure S20 Structure factor after carbamate-type reaction

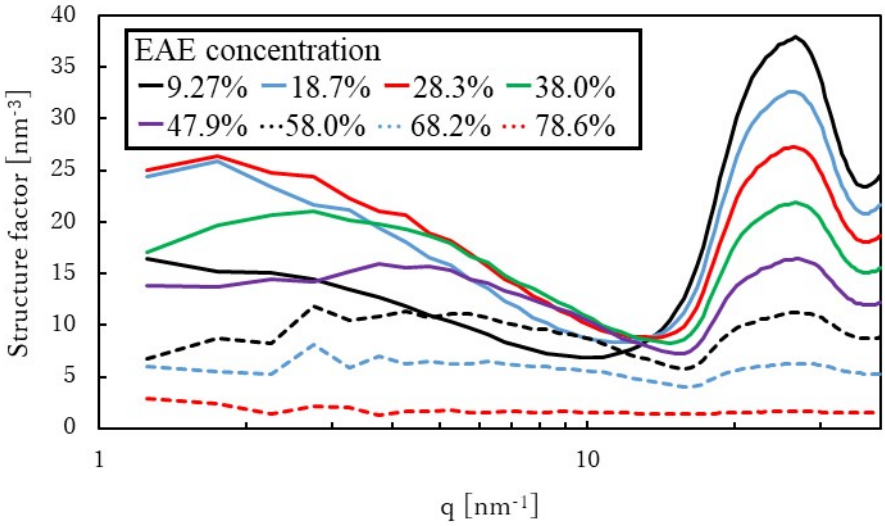

Figure S21 Structure factor after bicarbonate-type reaction (all)

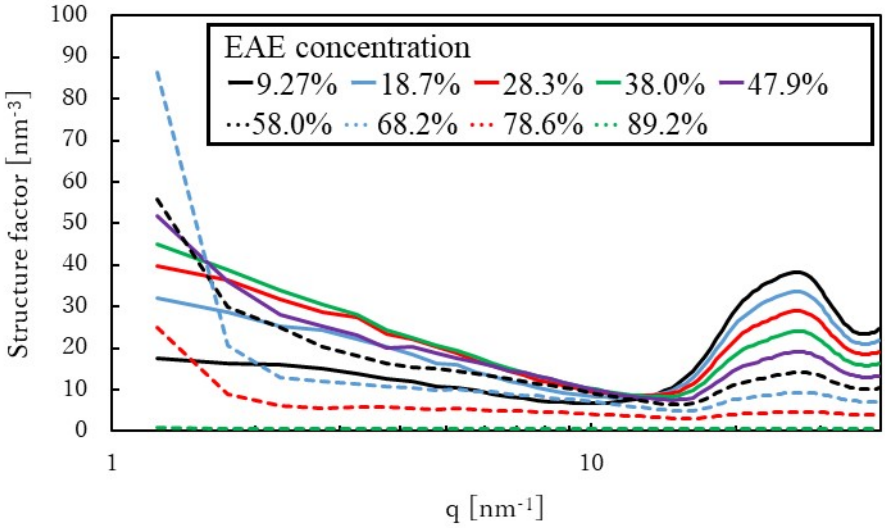

Figure S22 Structure factor after bicarbonate-type reaction (half)

Table S2 The q values (in nm^{-1}) used for evaluation of concentration fluctuation in each solution

EAE [wt%]	Before absorption	Carbamate	Bicarbonate (all)	Bicarbonate (half)
0	1.341	1.341	1.341	1.341
9.27	1.346	1.348	1.351	1.348
18.7	1.351	1.354	1.357	1.355
28.3	1.355	1.359	1.363	1.361
38	1.359	1.364	1.367	1.366
47.9	1.363	1.369	1.370	1.371
58	1.367	1.374	1.370	1.374
68.2	1.370	1.377	1.372	1.376
78.6	1.373	1.380	1.340	1.377
89.2	1.376	1.378	-	1.376