Self-Diffusion Coefficients of the Binary H₂O – CO₂ Mixture at High Temperatures and Pressures

Supporting Information

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Table S-1. Density of TIP4P/2005 H_2O and Self-Diffusion Coefficient of EPM2 CO_2 in H_2O.

T/K	P/MPa	Density$_{NIST}$/ (kg·m^{-3})	Density$_{MD}$/ (kg·m^{-3})	% Absolute deviation	Diffusion coefficient of CO_2 in H_2O / (10^{-9} m^2·s^{-1})
323.15	250	1075.1	1078 ± 5	0.27	2.4 ± 0.3
323.15	500	1136.7	1141 ± 5	0.38	2 ± 0.2
323.15	750	1185.2	1190 ± 4	0.40	1.7 ± 0.1
323.15	1000	1225.7	1229 ± 4	0.27	1.4 ± 0.2
423.15	250	1018	1019 ± 6	0.10	6.8 ± 0.6
423.15	500	1083.7	1087 ± 5	0.30	5.6 ± 0.5
423.15	750	1134.6	1138 ± 5	0.30	4.6 ± 0.4
423.15	1000	1176.8	1180 ± 5	0.27	4.1 ± 0.4
523.15	250	947.74	946 ± 7	0.18	13 ± 1
523.15	500	1025.6	1026 ± 6	0.04	10 ± 1
523.15	750	1082.4	1083 ± 5	0.06	8.9 ± 0.8
523.15	1000	1128.3	1129 ± 5	0.06	7.5 ± 0.9
623.15	250	867.82	864 ± 8	0.44	20 ± 2
623.15	500	964.13	962 ± 7	0.22	15 ± 2
623.15	750	1029.3	1028 ± 6	0.13	13 ± 1
623.15	1000	1080.1	1079 ± 6	0.10	11 ± 1
723.15	250	781.06	776 ± 8	0.65	29 ± 3
723.15	500	901.51	897 ± 7	0.50	21 ± 2
723.15	750	976.45	972 ± 6	0.46	17 ± 2
723.15	1000	1033	1029 ± 6	0.39	15 ± 1
823.15	250	691.2	686 ± 9	0.75	40 ± 4
823.15	500	839.41	833 ± 7	0.76	28 ± 3
823.15	750	924.93	918 ± 7	0.75	23 ± 2
823.15	1000	987.37	981 ± 6	0.65	19 ± 2
923.15	250	604.3	602 ± 9	0.38	51 ± 5
923.15	500	779.33	771 ± 8	1.07	35 ± 3
923.15	750	875.45	866 ± 7	1.08	28 ± 3
923.15	1000	943.77	934 ± 7	1.04	23 ± 2
1023.15	250	527.56	527 ± 9	0.11	63 ± 7
1023.15	500	722.46	714 ± 8	1.17	43 ± 4
1023.15	750	828.5	817 ± 7	1.39	34 ± 3
1023.15	1000	902.4	890 ± 7	1.37	29 ± 3

Table S-2. Density of EPM2 CO_2 and Self-Diffusion Coefficient of TIP4P/2005 H_2O in CO_2.

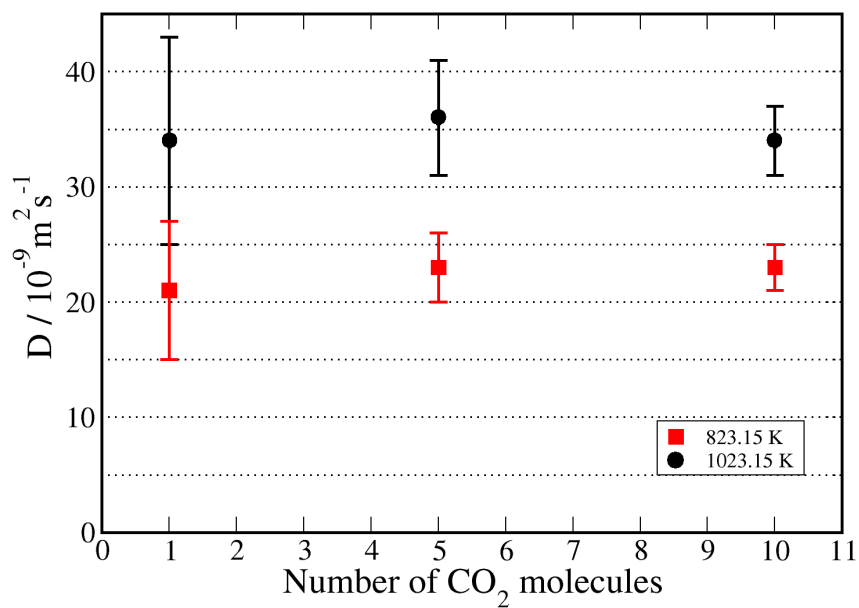| T/K	P/MPa	Density$_{NIST}$/ (kg·m^{-3})	Density$_{MD}$/ (kg·m^{-3})	% Absolute deviation	Diffusion coefficient of H_2O in CO_2 (10^{-9} m^2·s^{-1})
323.15	250	1248.3	1232 ± 2	1.31	6.8 ± 0.8
323.15	500	1390.8	1374 ± 1	1.21	4.3 ± 0.5
323.15	750	1484	1465 ± 1	1.28	2.9 ± 0.4
323.15	1000	n/a	1533 ± 1	n/a	2.2 ± 0.3
423.15	250	1121.9	1103 ± 2	1.68	16 ± 2
423.15	500	1295.6	1275 ± 2	1.59	10 ± 1
423.15	750	1403.2	1379 ± 1	1.72	7.2 ± 0.6
423.15	1000	n/a	1455 ± 1	n/a	5.7 ± 0.5
523.15	250	1016	996 ± 2	1.97	26 ± 2
523.15	500	1215.5	1191 ± 2	2.02	16 ± 1
523.15	750	1335.3	1305 ± 2	2.27	12 ± 1
523.15	1000	n/a	1388 ± 1	n/a	9.8 ± 0.9
623.15	250	927.46	907 ± 2	2.21	37 ± 3
623.15	500	1146.4	1119 ± 2	2.39	23 ± 2
623.15	750	1276.5	1242 ± 2	2.70	18 ± 2
623.15	1000	n/a	1330 ± 1	n/a	14 ± 1
723.15	250	853.19	833 ± 1	2.37	50 ± 4
723.15	500	1085.8	1057 ± 2	2.65	31 ± 3
723.15	750	1224.4	1186 ± 2	3.14	24 ± 2
723.15	1000	n/a	1279 ± 2	n/a	19 ± 2
823.15	250	790.37	771 ± 1	2.45	63 ± 6
823.15	500	1032	1002 ± 2	2.91	39 ± 3
823.15	750	1177.5	1137 ± 2	3.44	29 ± 3
823.15	1000	n/a	1233 ± 2	n/a	24 ± 2
923.15	250	736.7	718 ± 1	2.54	77 ± 7
923.15	500	983.92	954 ± 1	3.04	48 ± 4
923.15	750	1134.6	1092 ± 2	3.75	36 ± 3
923.15	1000	n/a	1191 ± 2	n/a	30 ± 3
1023.15	250	690.43	673 ± 1	2.52	91 ± 9
1023.15	500	940.66	911 ± 1	3.15	56 ± 5
1023.15	750	1095.3	1052 ± 2	3.95	43 ± 4
1023.15	1000	n/a	1153 ± 2	n/a	35 ± 3

Figure S-1. Self-diffusion coefficient of CO_2 in H_2O at 750 MPa, as a function of the number of solvent molecules used.
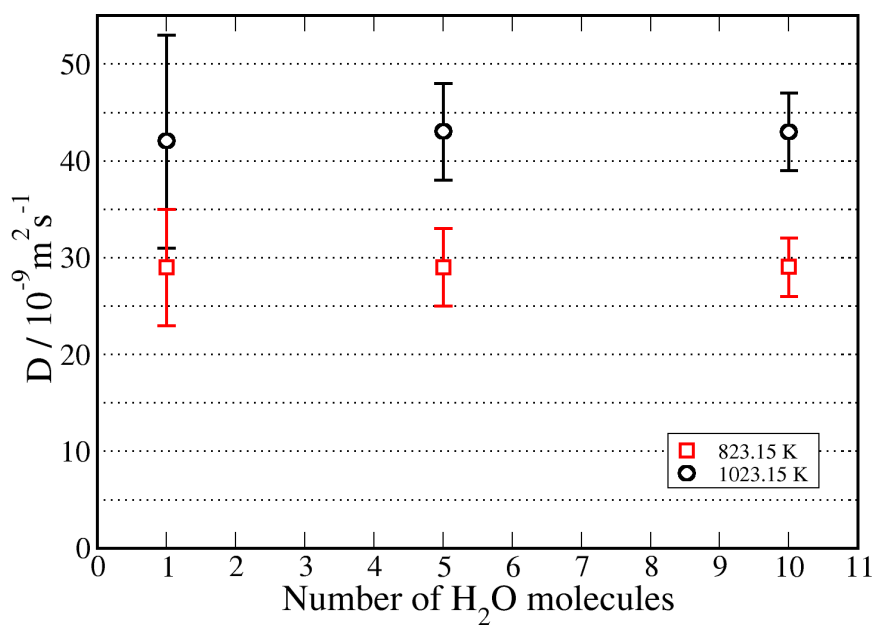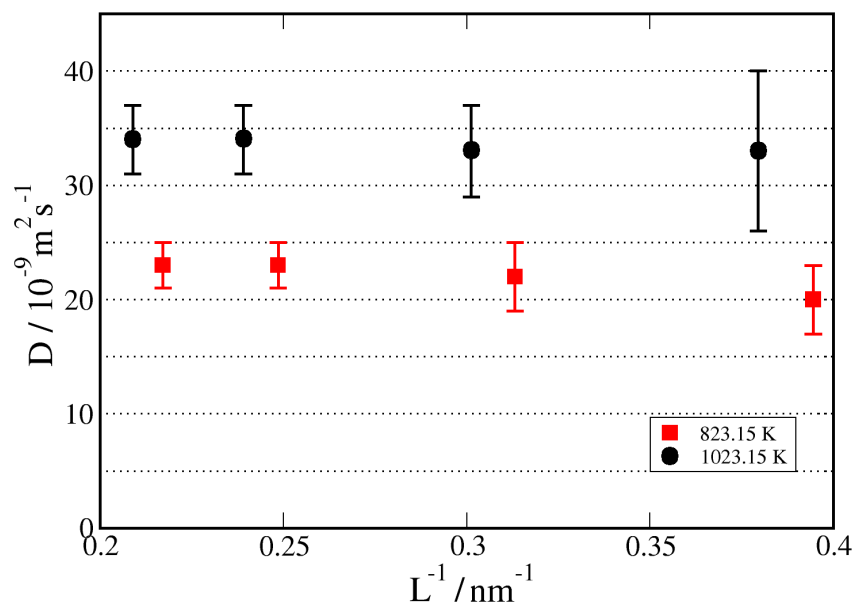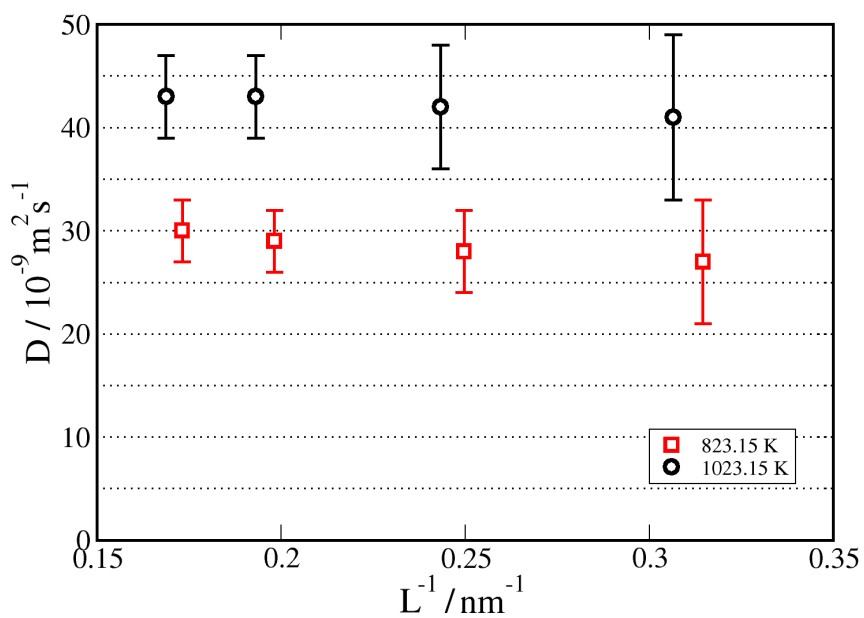

Figure S-2. Self-diffusion coefficient of H_2O in CO_2 at 750 MPa, as a function of the number of solvent molecules used.

(a)

(b)

Figure S-3. Self-diffusion coefficients as a function of the inverse simulation box length at 750 MPa for **(a)** CO_2 in H_2O, and **(b)** H_2O in CO_2.