Supplementary Information

Phase behaviour of liquid CO_2 with an impurity of water: Influence of CO_2 hydrate.

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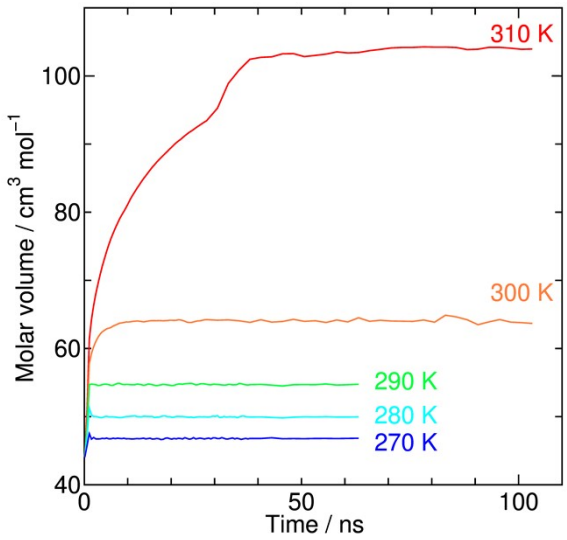

Fig. S1 Time evolution of the molar volume of liquid CO_2 averaged every 1 ns at a pressure of 10 MPa and at temperatures of (blue) 270, (cyan) 280, (green) 290, (orange) 300, and (red) 310 K.

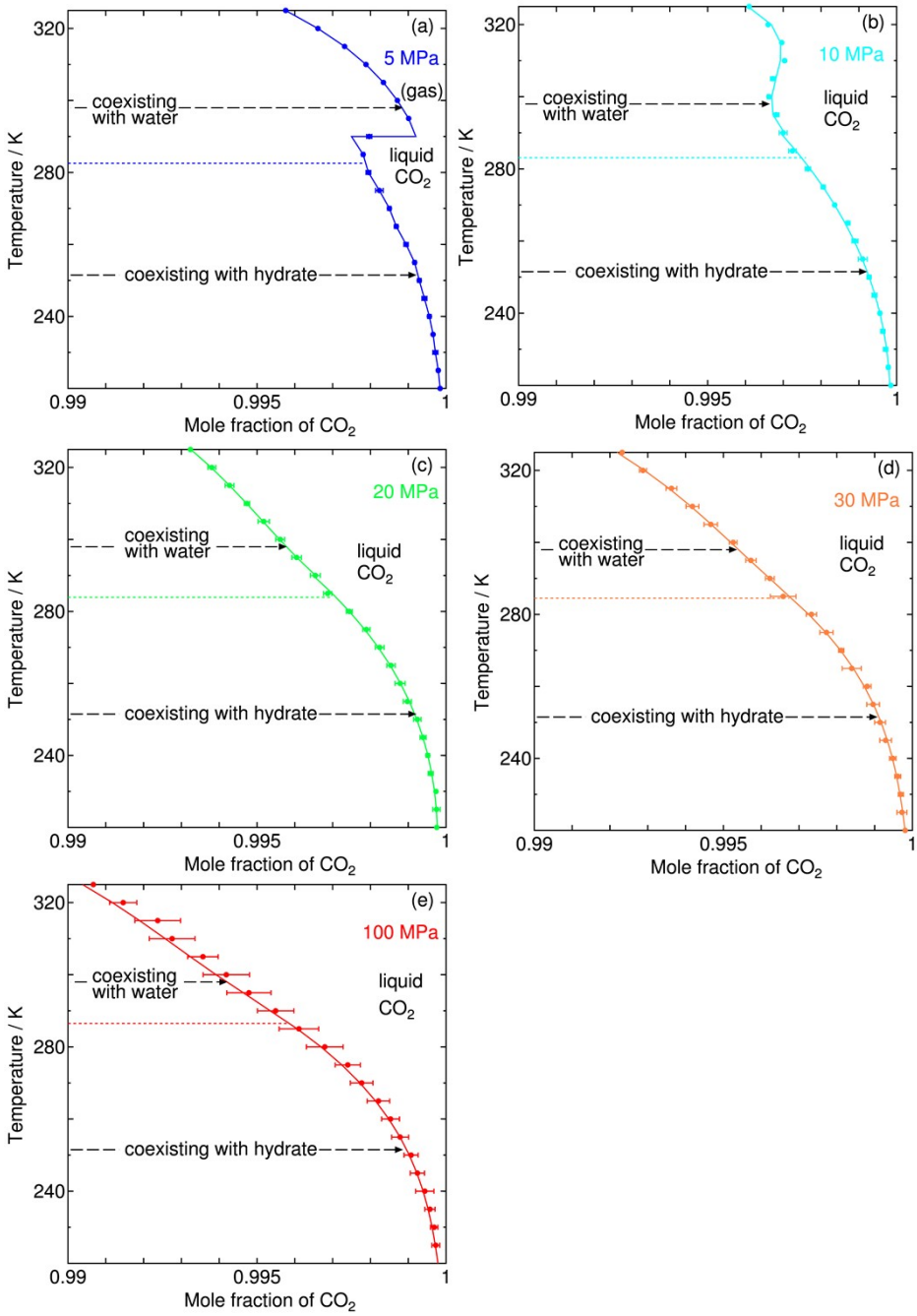

Fig. S2 Magnified phase diagram of the binary mixture of water and CO_2 for a region close to pure CO_2 at (a) 5, (b) 10, (c)20, (d) 30, and (e) 100 MPa. The stable region of fluid CO_2 is separated by the solid curve. Liquid CO_2 coexists with either the aqueous solution or CO_2 hydrate in the left region of each solid curve. Each dotted line indicates the dissociation temperature above which no hydrate is stable and the CO_2 fluid is in equilibrium with the aqueous solution. The blue line in panel (a) depicts the interpolated solubility curve taking account of the breaks due to the vaporization of liquid CO_2.