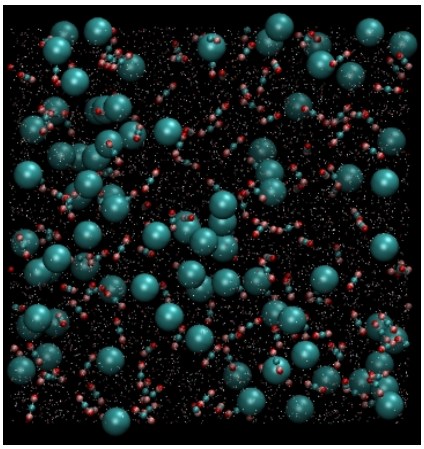
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

160 CO_2



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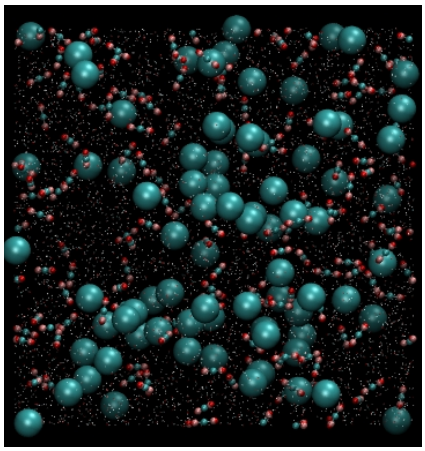

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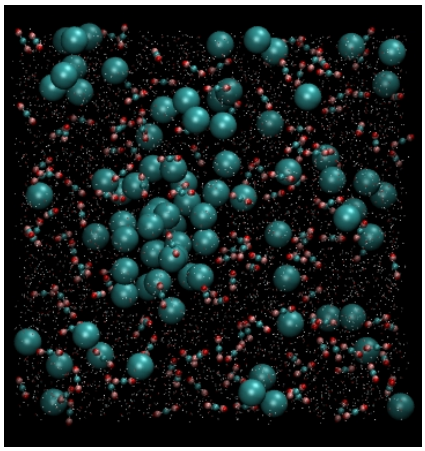

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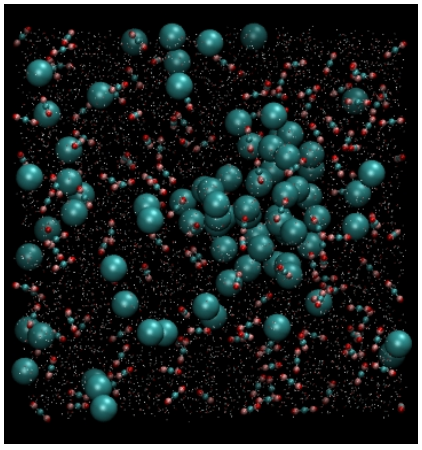

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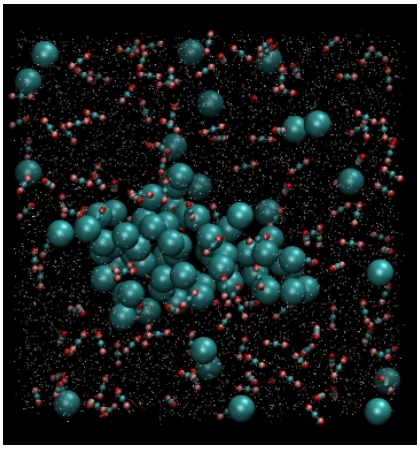

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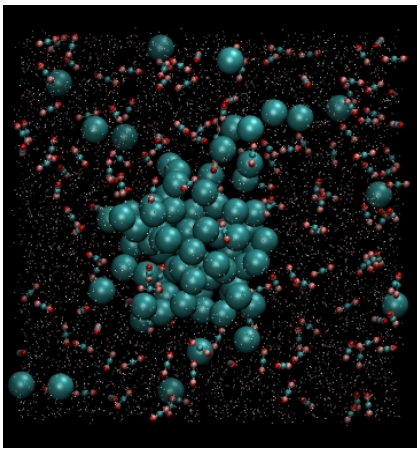

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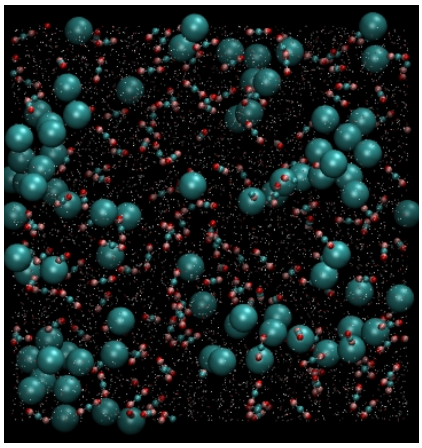
180 CO_2



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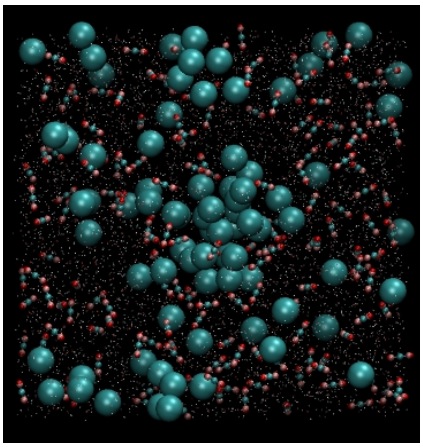

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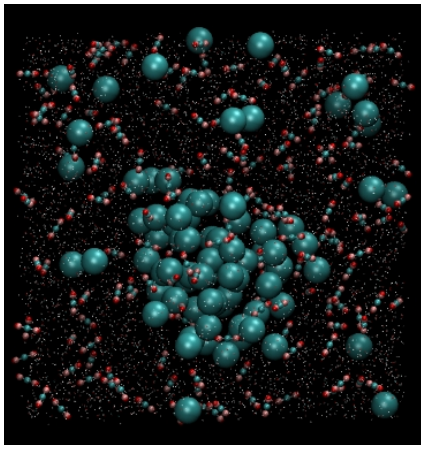

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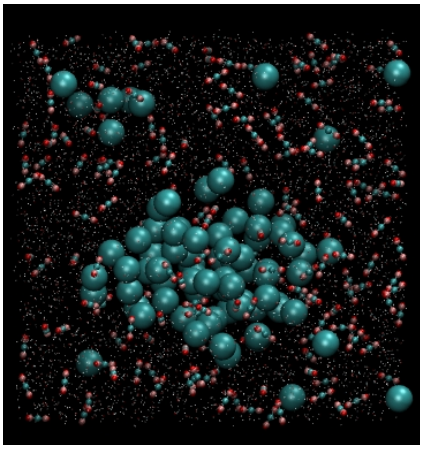

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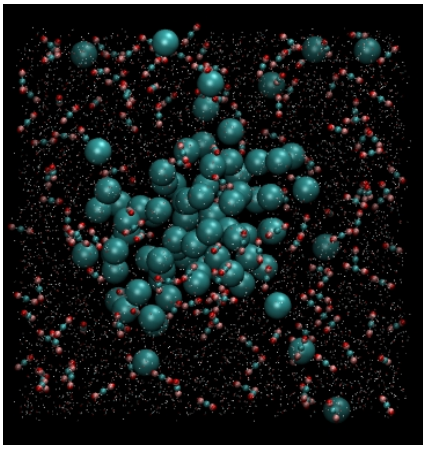

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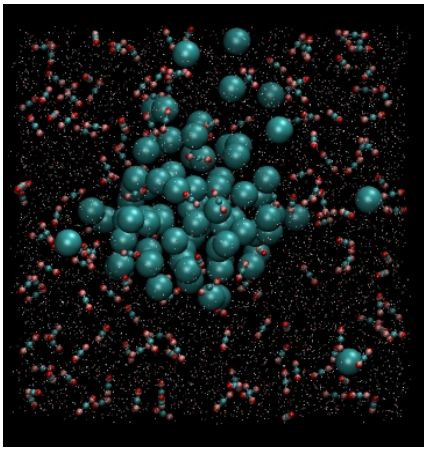

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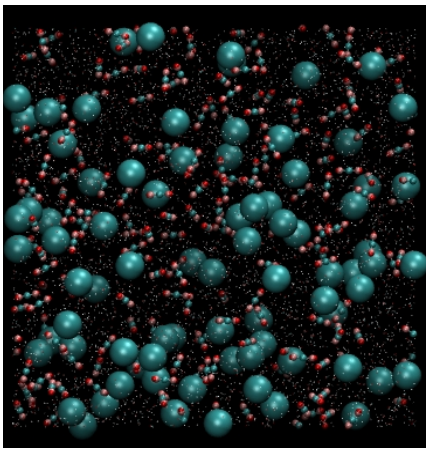
200 CO_2



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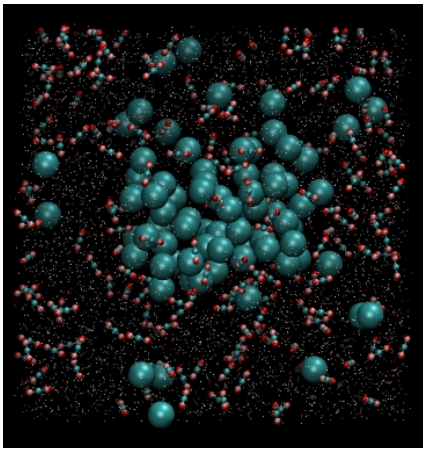

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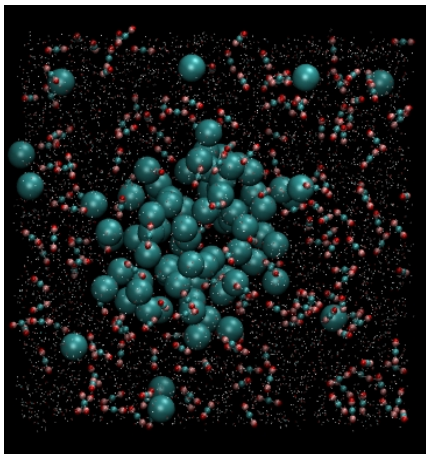

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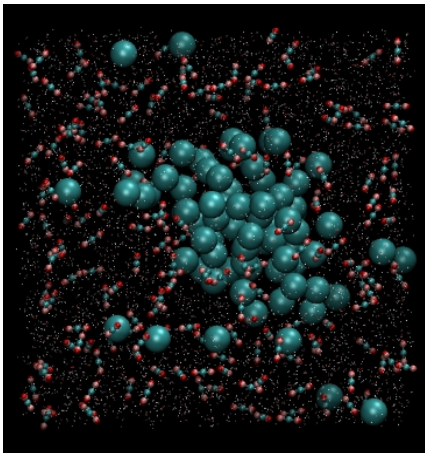

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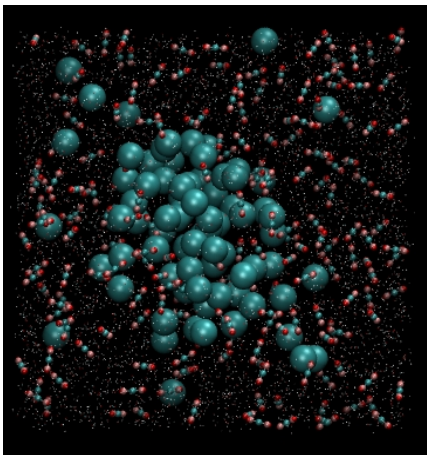

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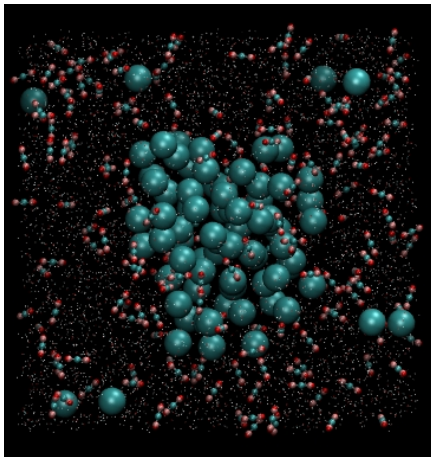

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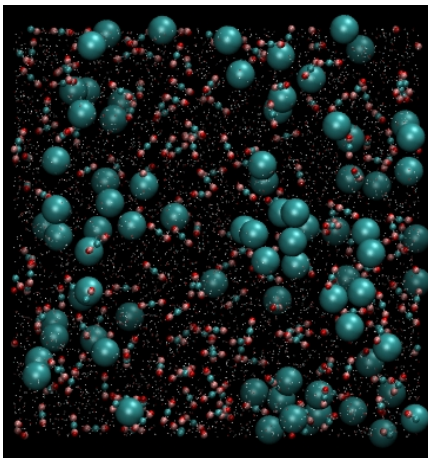
220 CO_2



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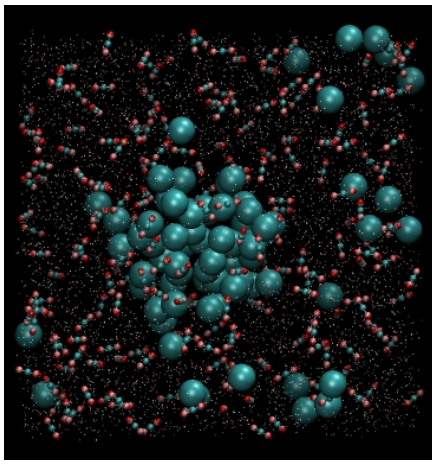

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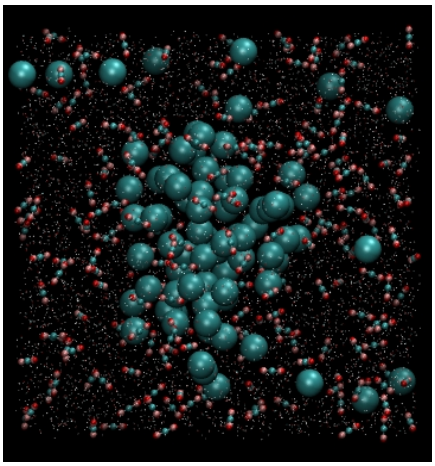

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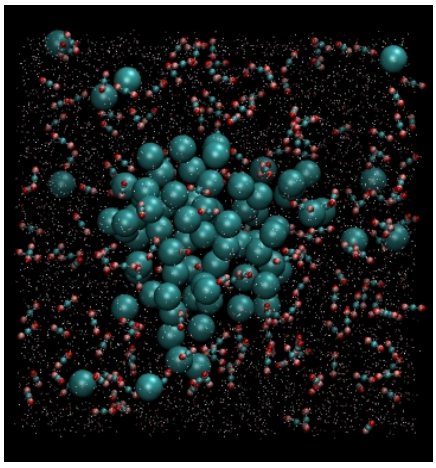

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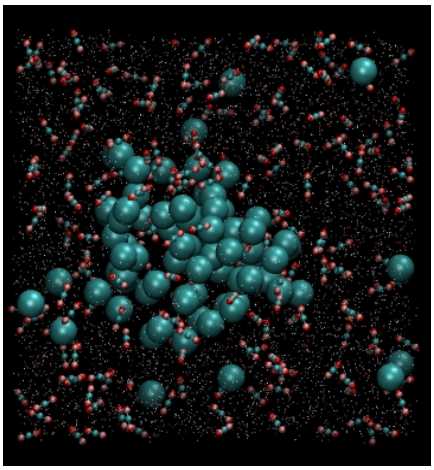

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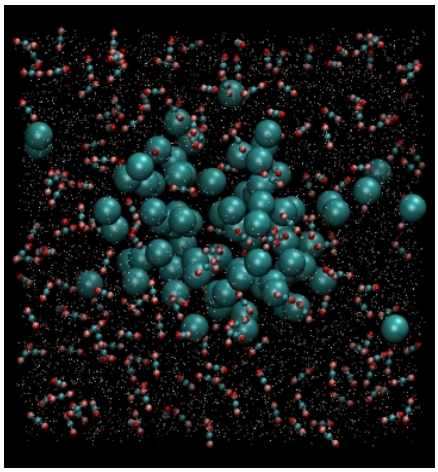

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240 CO_2

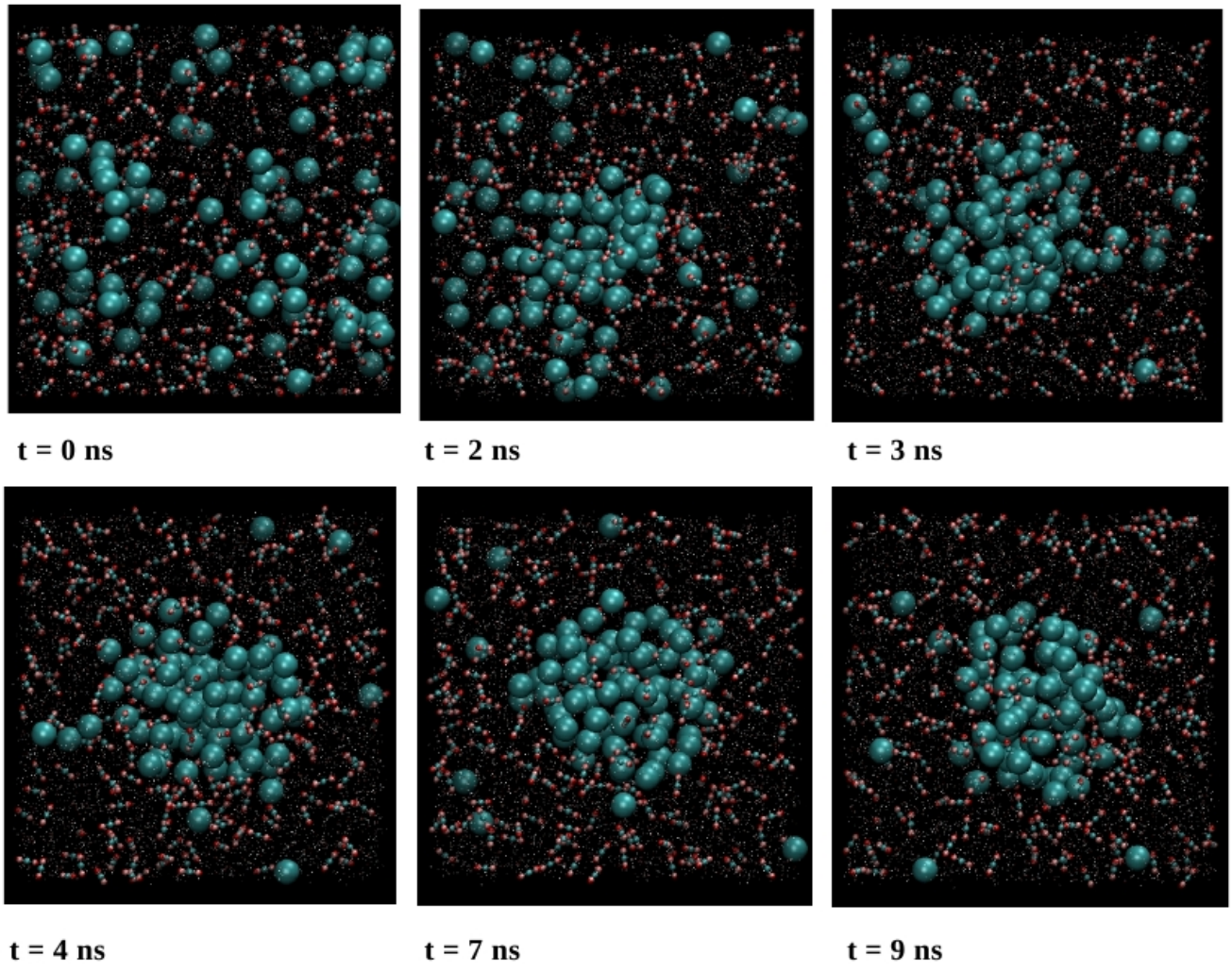


Figure S1: Bubble formation in the CH_4-CO_2-H_2O ternary system in the presence of various number of CO_2 molecules. Methane molecules are represented as large green dots, carbon dioxide by ball and stick model and water molecules are shown as small dots.

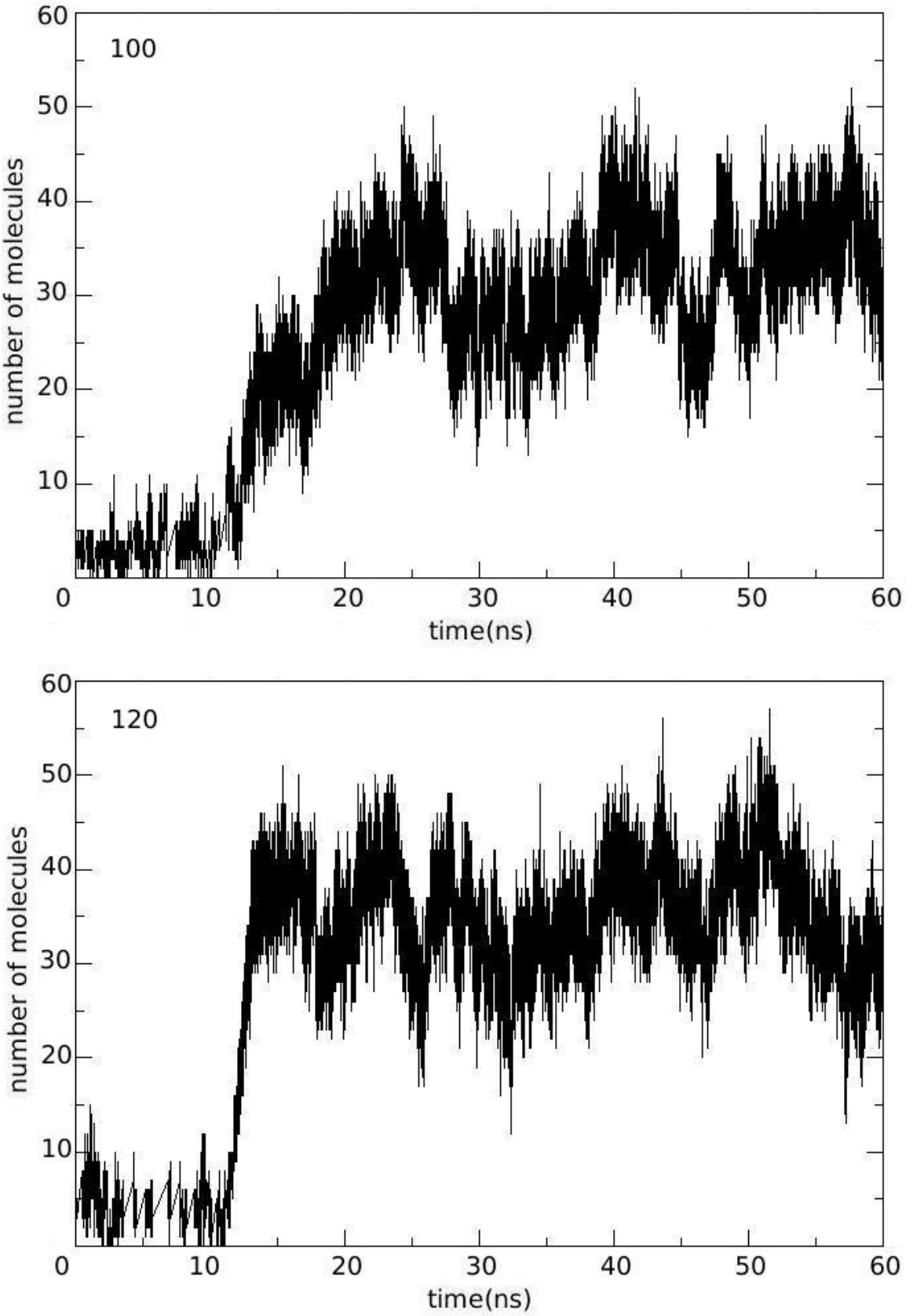
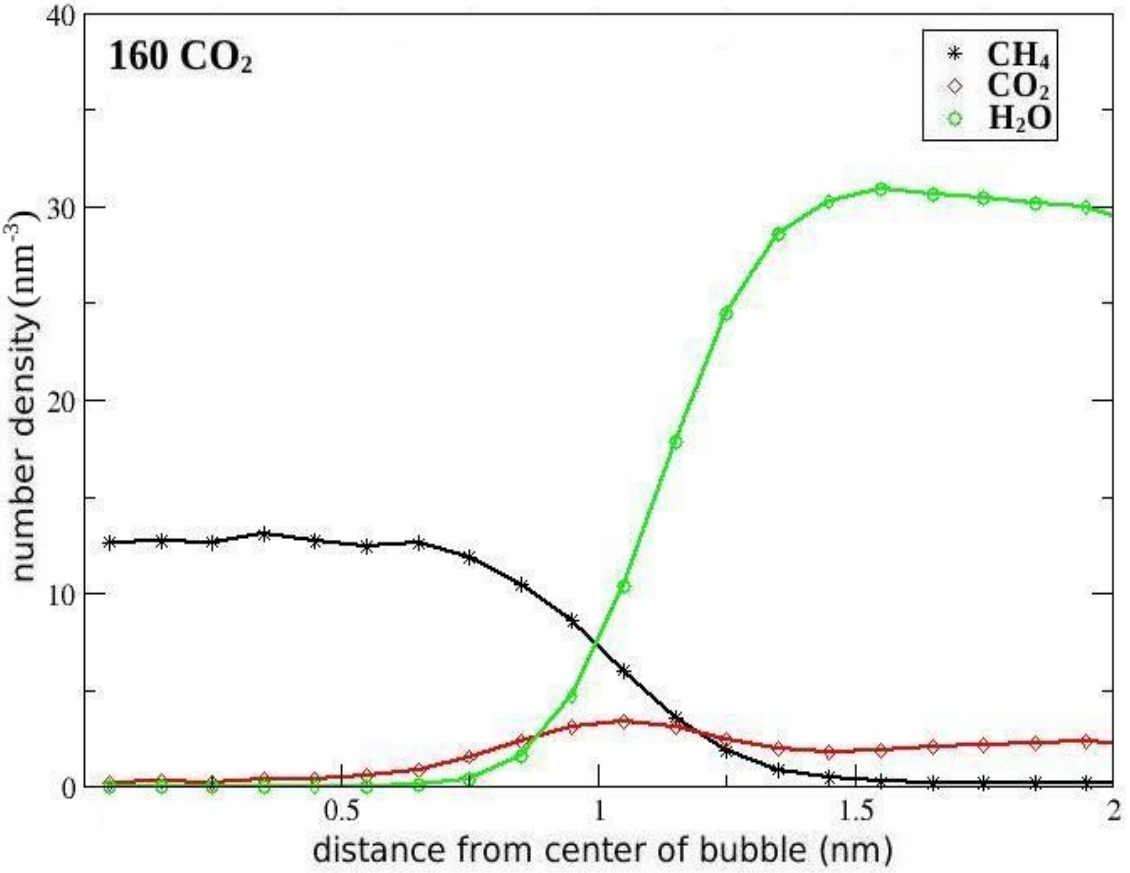
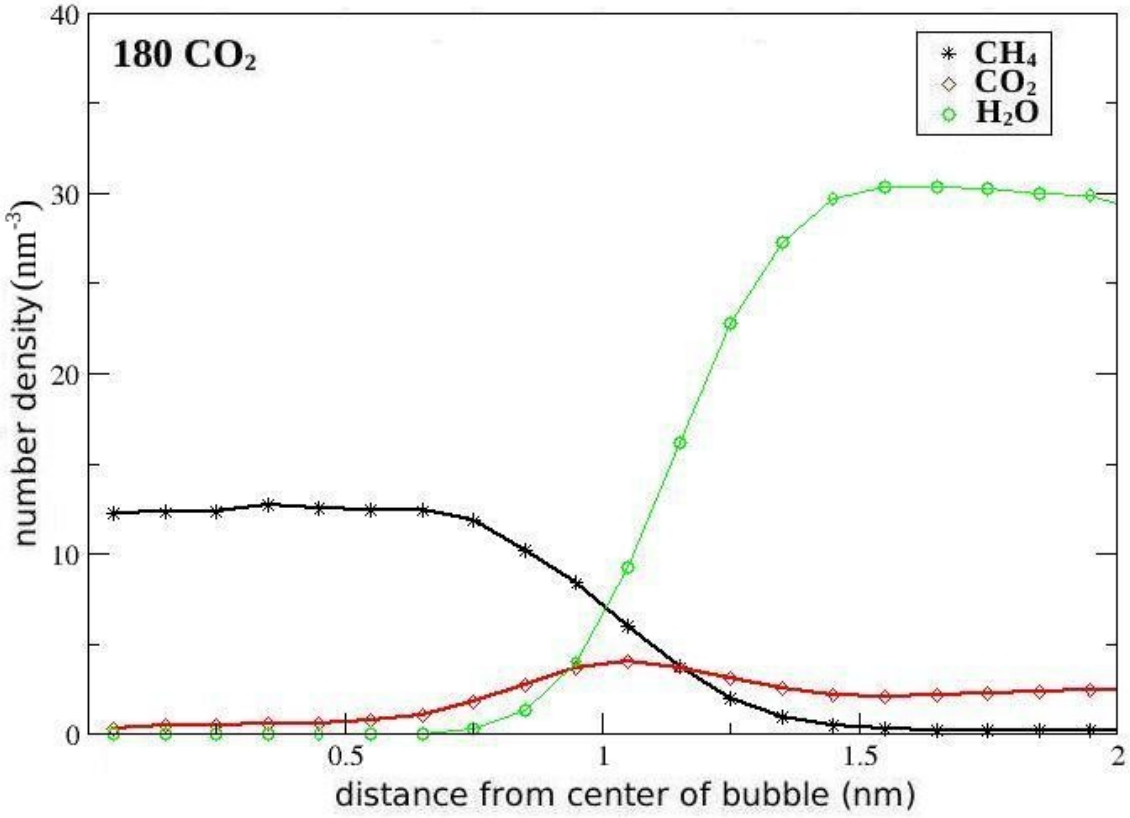


Figure S2 : The number of CH_4 molecules in the gas bubble as a function of time for the CH_4-CO_2-H_2O ternary systems with 100 and 120 CO_2 molecules.


160 CO2
CH4
CO2
H2O
number density (nm-3)
distance from center of bubble (nm)
0
10
20
30
40
0.5
1
1.5
2


180 CO2
CH4
CO2
H2O
number density (nm-3)
distance from center of bubble (nm)
0
10
20
30
40
0.5
1
1.5
2

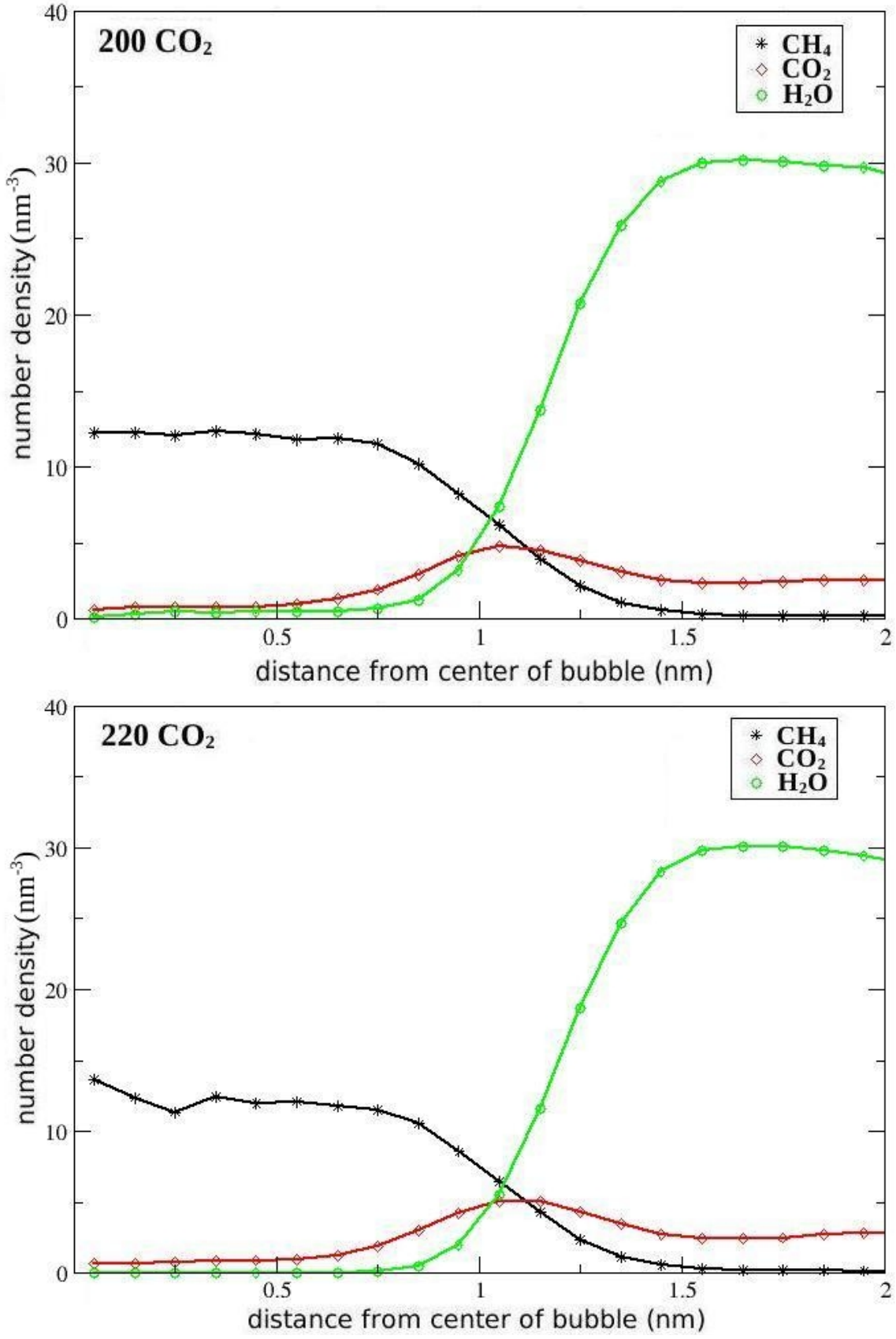


Figure S3 : The number density of CH_4, CO_2 and H_2O molecules as a function of distance from the center of the gas bubble for ternary systems with 160, 180, 200 and 220 CO_2 molecules.

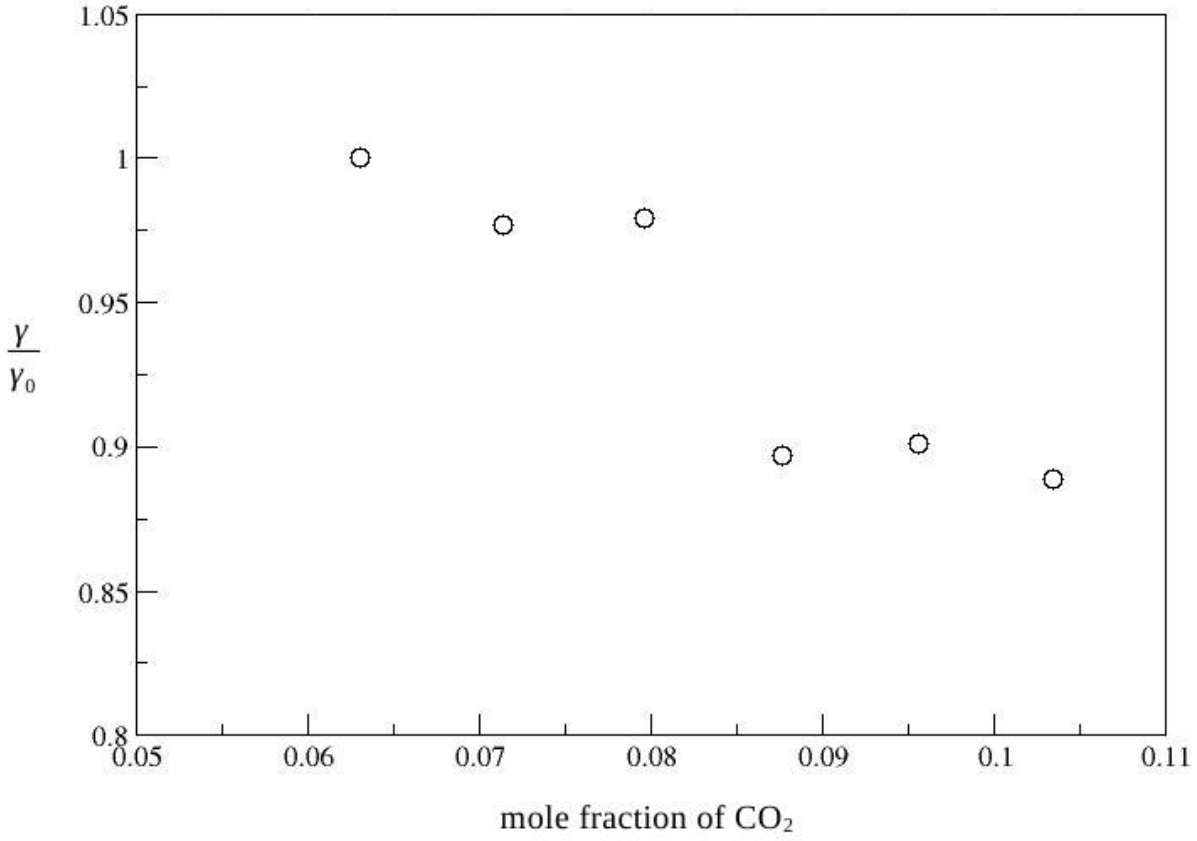


Figure S4: The relative surface tension at the bubble-water interface as a function of concentration of CO_2 in the ternary system.

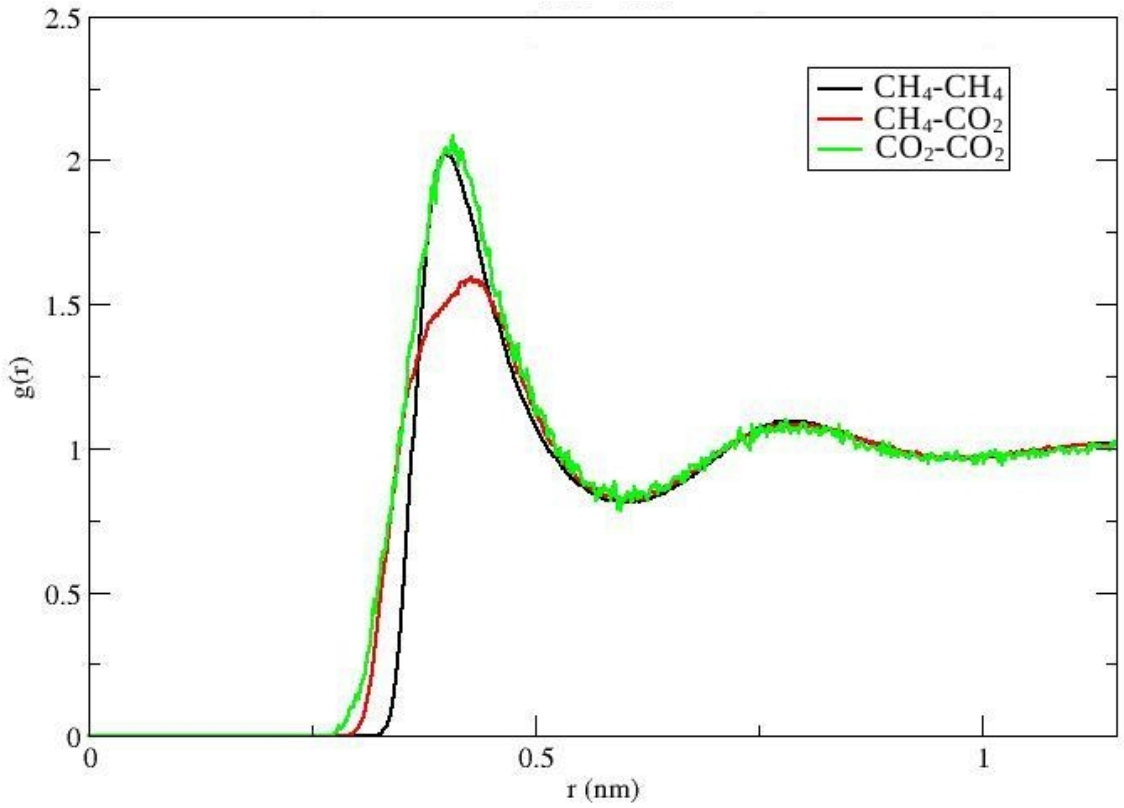


Figure S5: Radial distribution function for the CH_4-CH_4, CH_4-CO_2 and CO_2-CO_2 pair interactions in a dilute binary solution of CO_2 in super critical CH_4.