Supporting Information

Gate Opening, Diffusion and Adsorption of CO_2 and N_2 Mixtures in ZIF-8

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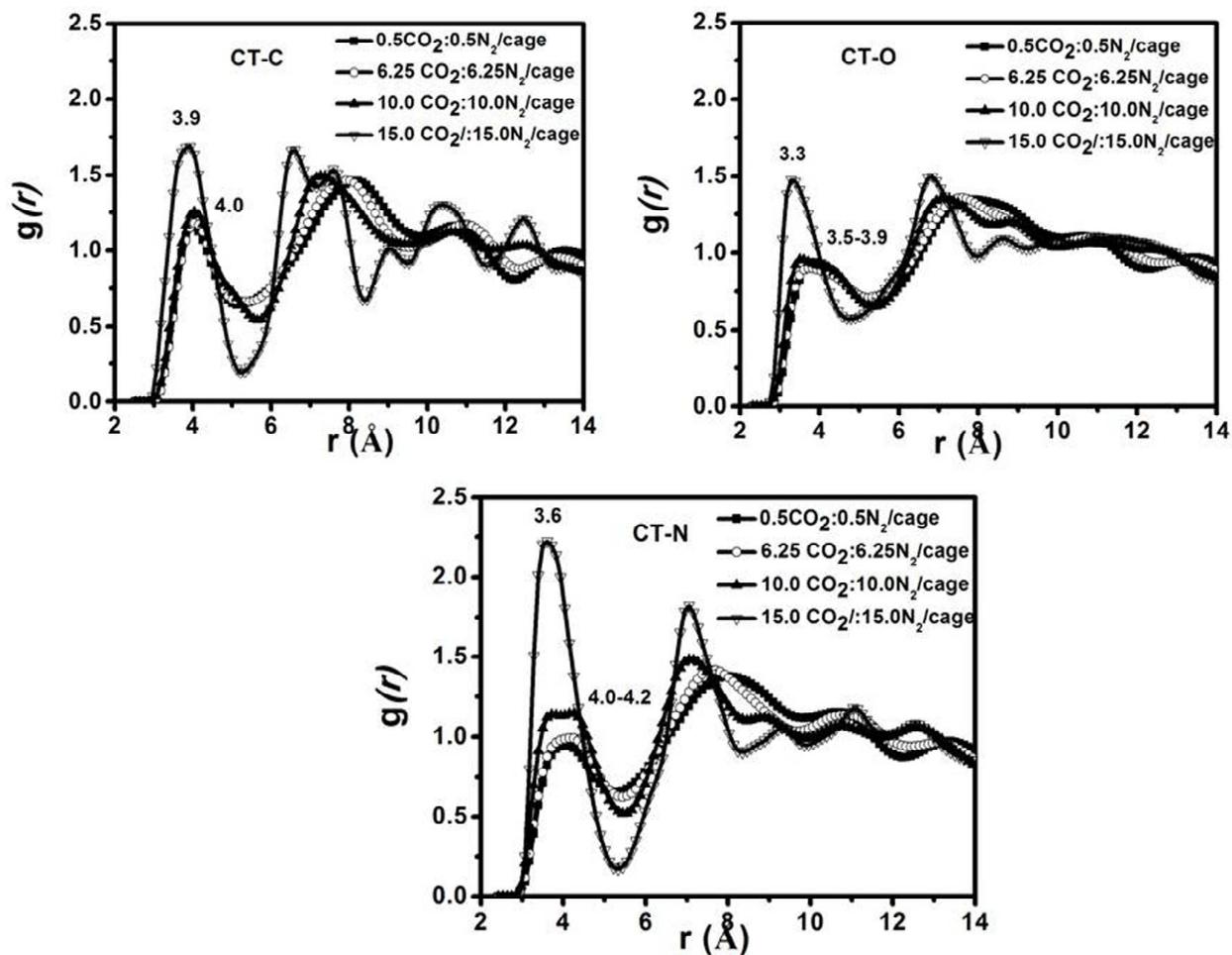
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Radial distribution functions (RDF's)

Radial distribution functions (RDF's) between atoms in guest molecules with lattice atoms and other atoms in gueast molecules are shown in the following figures.
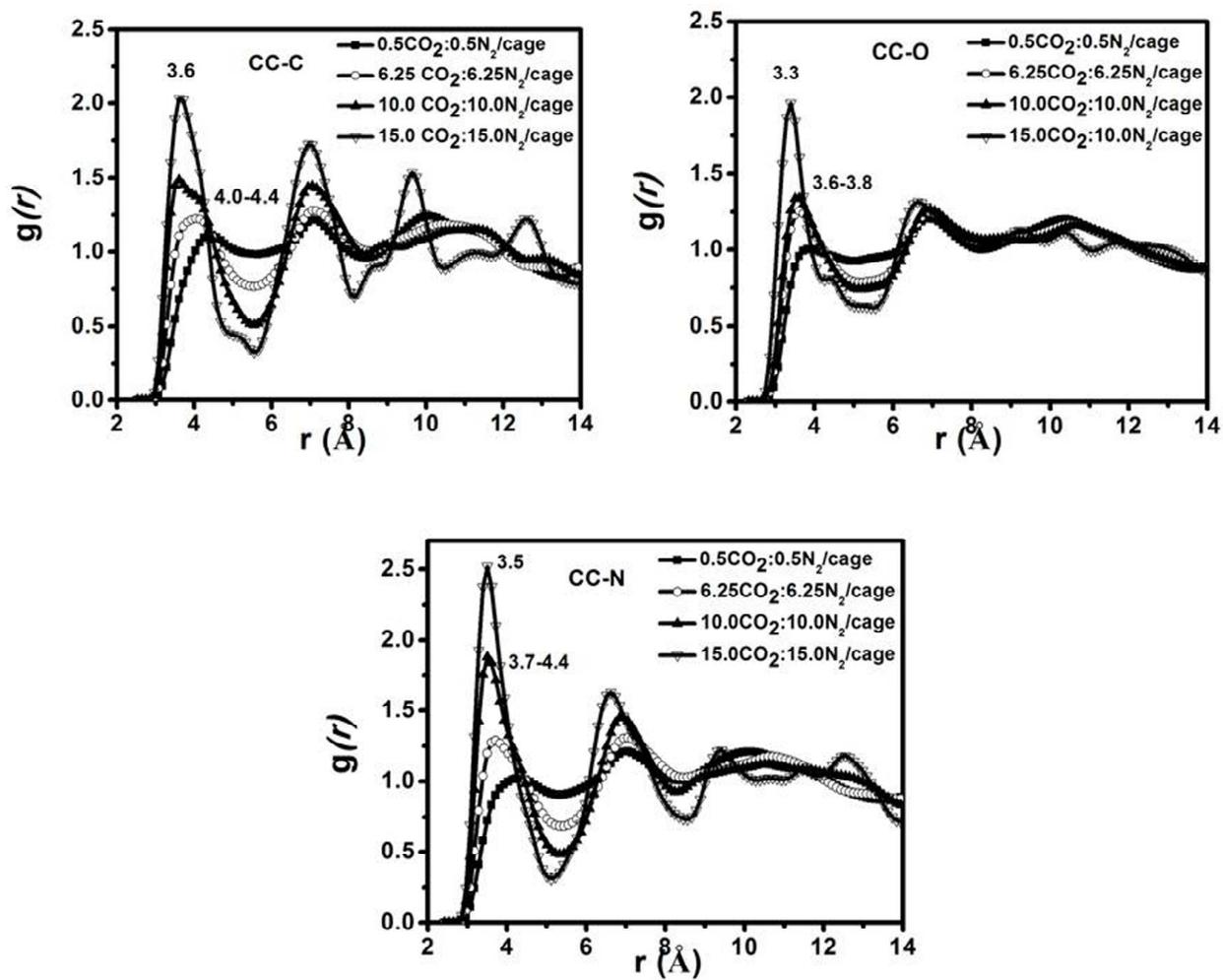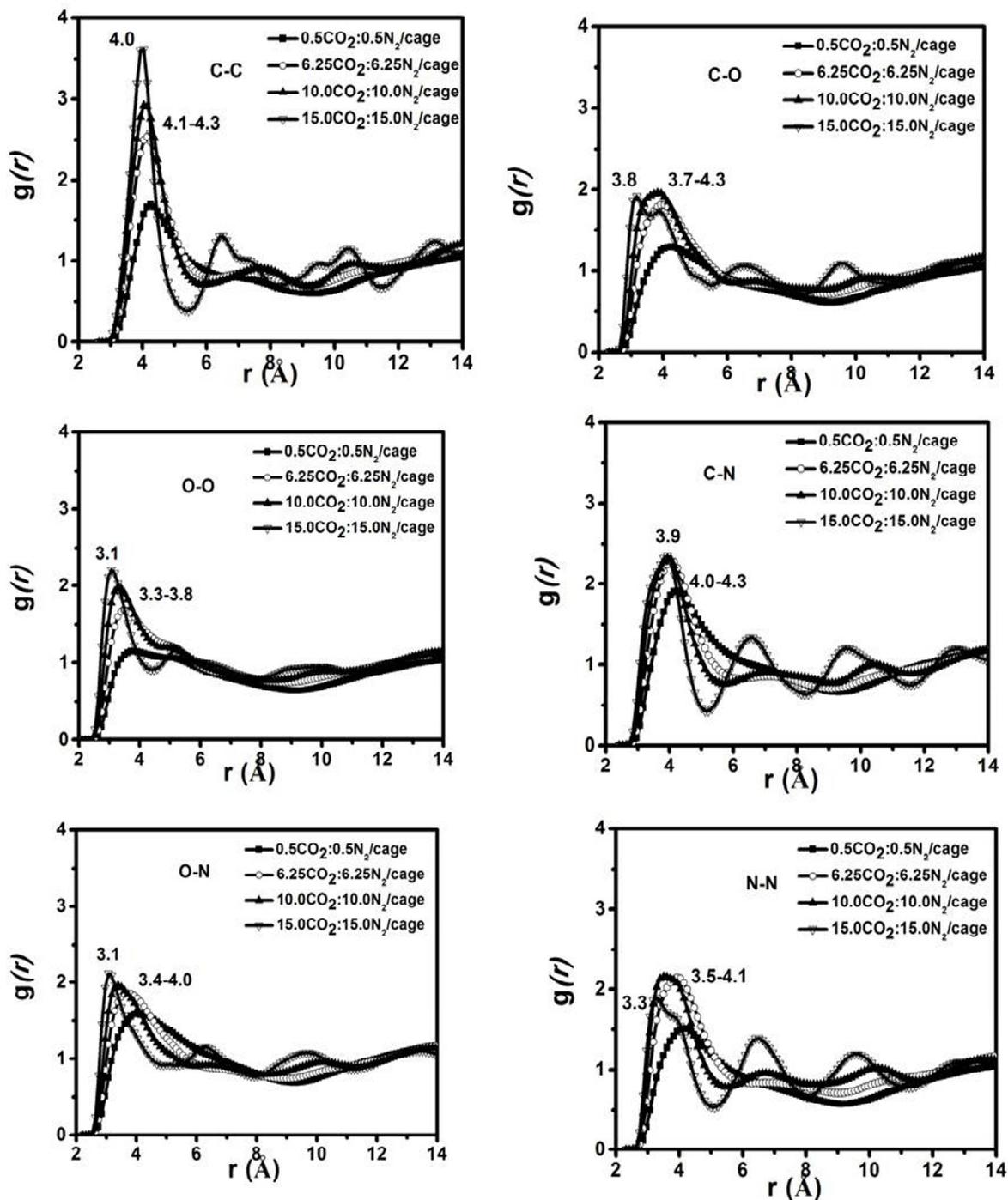
S1 The RDF of framework and guest between CC-C, CC-O and CC-N of mixture CO_2/N_2 when increasing loading.

S2 The RDF of framework and guest between CT-C, CT-O and CT-N of mixture CO_2/N_2 when increasing loading.
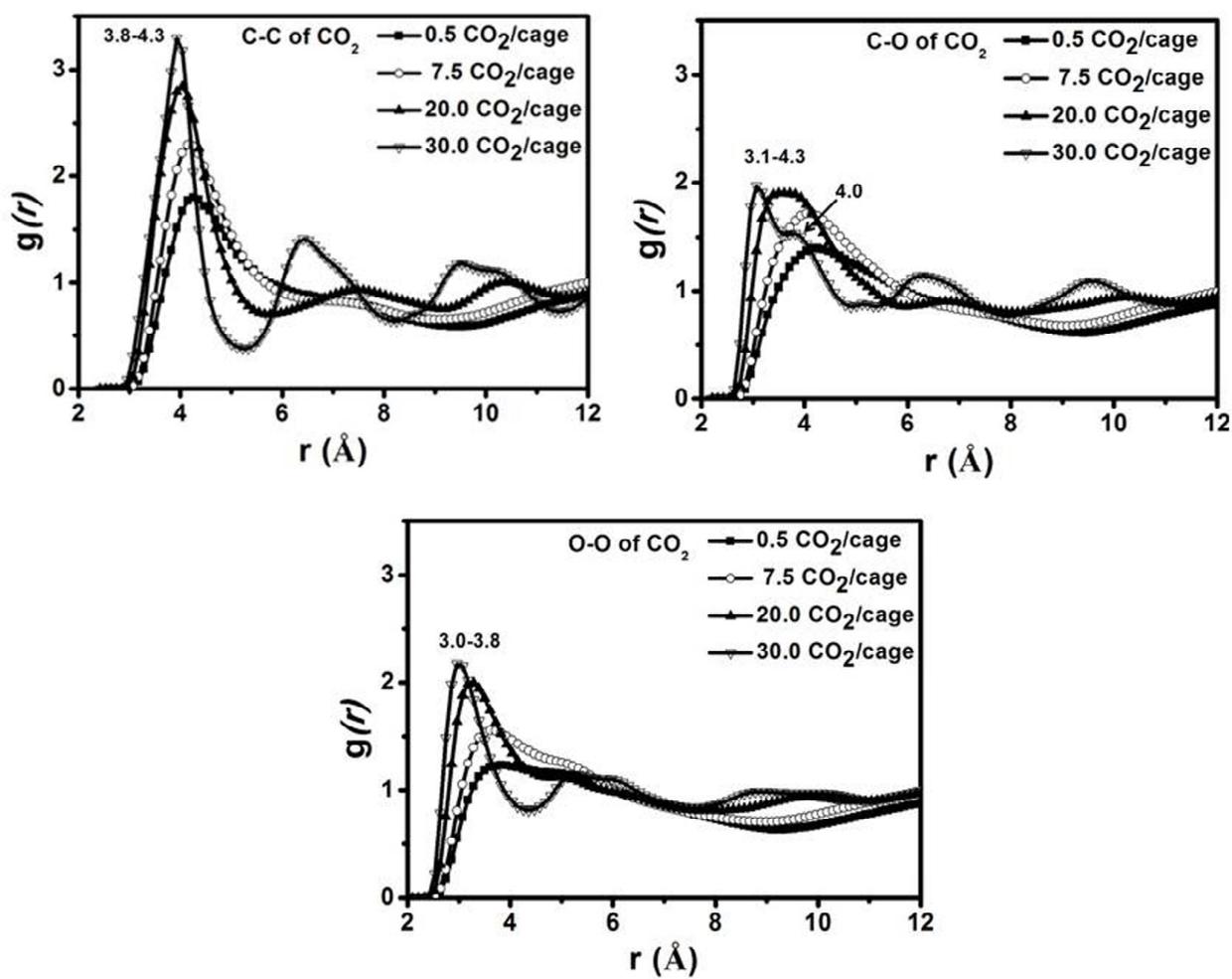
S3 The RDF between C-C, C-O and O-O of CO_2 in framework.

S4 The RDF between atoms belonging to different guest molecules in the mixture CO_2/N_2 in ZIF-8 for different loadings.

Self diffusion coefficients and diffusion selectivities

Loading concentration	D_s of mixture CO_2/N_2		$\alpha_{ij}^{diffusion}$
	CO_2	N_2	
1.25 (0.625 CO_2, 0.625 N_2)	2.905E-10	3.357E-10	0.865
2.5 (1.25 CO_2, 1.25 N_2)	3.361E-10	4.528E-10	0.742
5 (2.5CO_2, 2.5 N_2)	2.9153E-10	3.544E-10	0.823
7.5 (3.25 CO_2, 3.25N_2)	2.9045E-10	5.046E-10	0.576
10 (5 CO_2, 5 N_2)	3.381E-10	6.059E-10	0.558
12.5 (6.25CO_2, 6.25N_2)	3.733E-10	7.2907E-10	0.512
15 (7.5CO_2, 7.5N_2)	7.391E-10	9.1E-10	0.812

Table S1: Self diffusion coefficient D_s values in m^2/s shown in Fig. 3 and resulting diffusion selectivities for different equimolar concentrations. The concentration is given in molecules per cage, the diffusivity in m^2/s.