Supporting Information

Molecular Selectivity of CO-N_2 Mixed Hydrates: Raman Spectroscopy and GCMC Studies

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Content

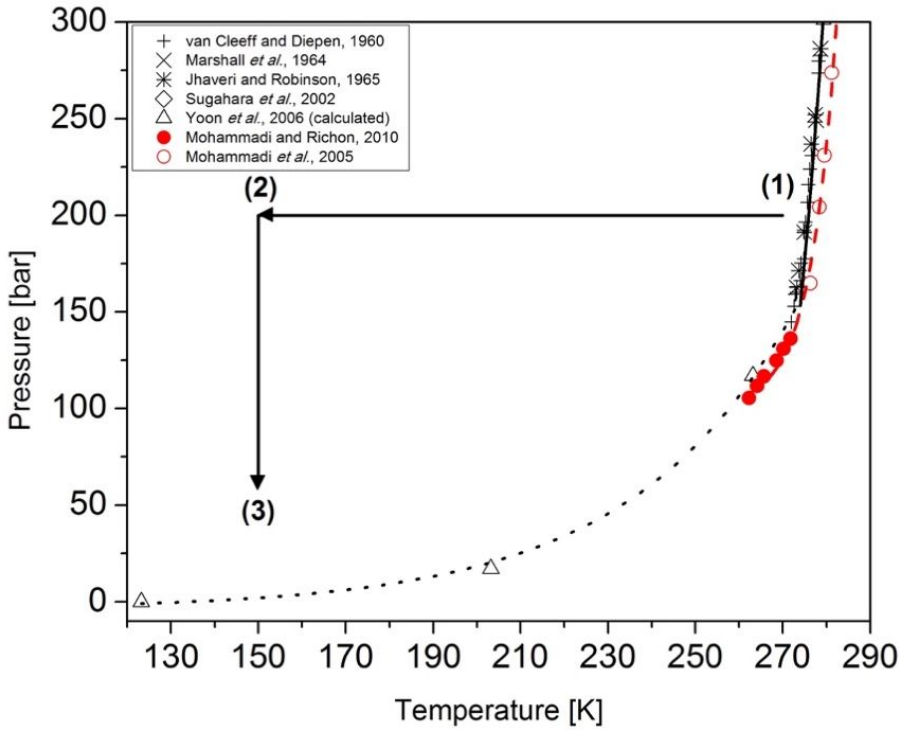

Figure S1: Phase diagram of pure CO and N_2 gas hydrates. The lines at 150 K and 200 bar represent the thermodynamic histories studied.

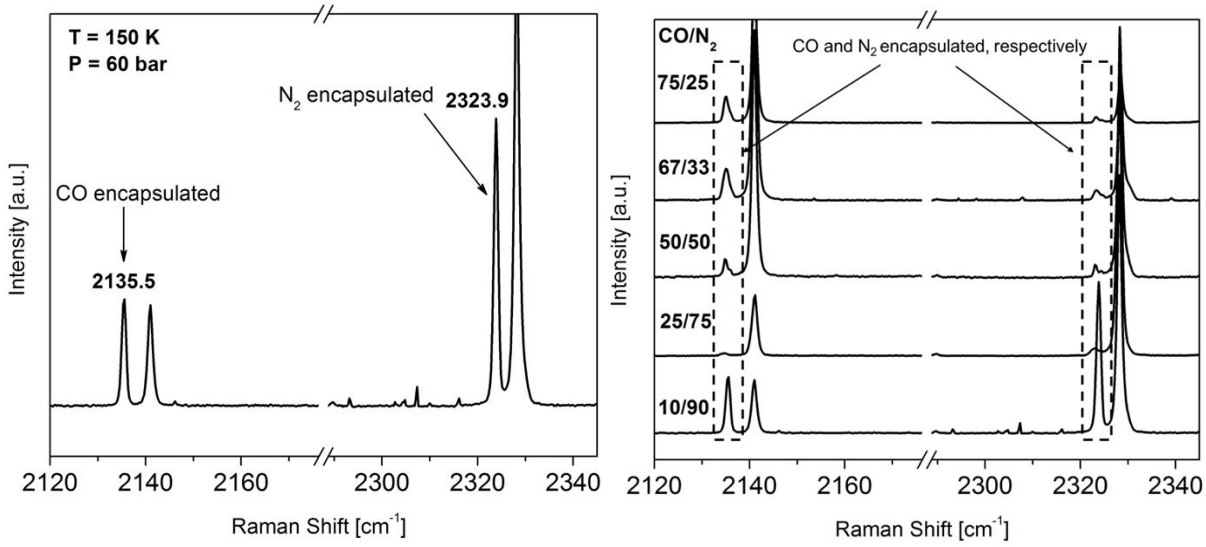

Figure S2: Raman signatures of the guest molecules encapsulation at 150 K and 60 bar for 10% of CO (left) and for all gas mixture composition (right).

H_2O	r_{OH}	r_{OM}	$\widehat{HOH}$	σ	ε	q
	0.9572	0.1250	104.52°			
O				3.16435	81.90	0.0
H				0.0	0.0	0.52422
M				0.0	0.0	-1.04844
CO	r_{CO}	$r_{CQ_{ext1}}$	$r_{OQ_{ext2}}$	σ	ε	q
	1.1282	0.4374	0.158			
C				3.385	39.89	0.831
O				2.885	61.57	0.0
Q_{ext1}				0.0	0.0	-0.636
Q_{ext2}				0.0	0.0	-0.195
N_2		r_{NN}	$\widehat{NN}$	σ	ε	q
		1.10	180°			
N				3.31	36.0	-0.482
CoM				0.0	0.0	0.964

Table S1: Description of the models used in the GCMC simulations for the H_2O, CO, and N_2 molecules. Energy terms ε are in given in K, distances r and σ in Å, and charges q in atomic units. CoM is the center of mass.