t0

t2

t5

Vapor peak intensity

100
80
60
40
20
0

LC CH4 intensity

800
600
400
200
0

SC CH4 intensity

300
200
100
0

Cage occupancy θ_S

0.9
0.8
0.7
0.6
0.5

Hydration number nc

6.8
6.6
6.4
6.2
6
5.8