

## Tables

Table 1 calculation conditions

Calculation conditions			Number of cages and molecules		
Solver	GROMACS 5.1.4		CO <sub>2</sub> molecule	-	1647
Boundary condition	-	Periodic	H <sub>2</sub> O molecule	-	9910
Step time	fs	2	Small cage	-	1450
Duration	ns	50	Large cage	-	1158
Ensemble	-	NPT	<b>Model</b>		
Pressure	MPa	6	CO <sub>2</sub>	-	OPLS-AA
Temperature	K	200, 240, 280	H <sub>2</sub> O	-	TIP4P/ice