

Supporting Information

Cage Fusion from Bi-Cage to Tri-Cage during Nucleation of Methane Hydrate: DFT-D simulation

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Table SI. The bond length of CH₄ in mono-cage.

Cage	Atom		Bond length (Å)	Average bond length (Å)
18	C	H1	1.091	1.092
	C	H2	1.092	
	C	H3	1.092	
	C	H4	1.093	
20	C	H1	1.093	1.094
	C	H2	1.094	
	C	H3	1.094	
	C	H4	1.094	
22	C	H1	1.095	1.095
	C	H2	1.095	
	C	H3	1.095	
	C	H4	1.095	
24	C	H1	1.096	1.097
	C	H2	1.097	
	C	H3	1.097	
	C	H4	1.097	