Supporting Information

Cavity Closure Dynamics of Peracetylated β-Cyclodextrins in Supercritical Carbon Dioxide.

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- Atomic charges used in the simulations.

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Atomic charges used in the simulations

Atomic charges were obtained by performing a RESP fitting along the lines presented in Appendices C and D of the Amber manual, version6. The atom labels are defined in Figure 2 of the paper.

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O2      OS  -0.427543
O3      OS  -0.493327
O6      OS  -0.461794
C7      C    0.711403
O7      O   -0.552784
C8      C    0.751747
O8      O   -0.556151
C9      C    0.814971
O9      O   -0.575642
C10     CT  -0.024815
H(C10)  H1   0.000000
C11     CT   0.000631
H(C11)  H1   0.000000
C12     CT  -0.001696
H(C12)  H1   0.000000
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