

SimulationType MonteCarlo
NumberOfCycles 10000
NumberOfInitializationCycles 5000
PrintEvery 500

CutOff 12.0

Forcefield Dubbeldam2007FlexibleIRMOF-1

Framework 0
FrameworkName IRMOF-1

UseChargesFromCIFFile yes
UnitCells 1 1 1
ExternalTemperature 300.00

ComputeEnergyHistogram yes
WriteEnergyHistogramEvery 100
EnergyHistogramSize 400
EnergyHistogramLowerLimit -1000
EnergyHistogramUpperLimit 1000

Component 0 MoleculeName methane
MoleculeDefinition TraPPE
TranslationProbability 1.0
RotationProbability 1.0
ReinsertionProbability 1.0
CreateNumberOfMolecules 1