

SimulationType MonteCarlo
NumberOfCycles 10000
NumberOfInitializationCycles 5000
PrintEvery 500
RestartFile no

Forcefield Dubbeldam2007FlexibleIRMOF-1

Framework 0
FrameworkName IRMOF-1
UnitCells 2 2 2
HeliumVoidFraction 0.82
ExternalTemperature 385
ExternalPressure 9.0e5

Component 0 MoleculeName argon
MoleculeDefinition TraPPE
MolFraction 0.40
TranslationProbability 0.5
RegrowProbability 0.5
IdentityChangeProbability 1.0
NumberOfIdentityChanges 2
IdentityChangeList 0 1
ReinsertionProbability 1.0
SwapProbability 1.0
CreateNumberOfMolecules 0

Component 1 MoleculeName methane
MoleculeDefinition TraPPE
MolFraction 0.60
TranslationProbability 0.5
RegrowProbability 0.5
IdentityChangeProbability 1.0
NumberOfIdentityChanges 2
IdentityChangeList 0 1
ReinsertionProbability 1.0
SwapProbability 1.0
CreateNumberOfMolecules 0