```
SimulationType                 MonteCarlo
NumberOfCycles                 10000
NumberOfInitializationCycles   5000
PrintEvery                     1000
ContinueAfterCrash             no


Forcefield                     Dubbeldam2007FlexibleIRMOF-1


Framework 0
FrameworkName IRMOF-1
UnitCells 1 1 1
HeliumVoidFraction 0.826
ExternalTemperature 300
ExternalPressure 0.70e5


Box 1
BoxLengths 246.0 246.0 246.0
CutOffCoulomb 50
ExternalTemperature 300
ExternalPressure 0.70e5

VolumeChangeProbability 0.2

Component 0 MoleculeName              methane
            MoleculeDefinition        TraPPE
            TranslationProbability    0.5
            RotationProbability       0.5
            ReinsertionProbability    0.5
            GibbsSwapProbability      1.0
            CreateNumberOfMolecules   0 100
```