```
SimulationType                MolecularDynamics
NumberOfCycles                10000
NumberOfEquilibrationCycles   5000
NumberOfInitializationCycles  5000
PrintEvery                    100
RestartFile                   no

Ensemble                      NVT

ChargeMethod                  Ewald
CutOff                        12.0
TimeStep                      0.0005
Forcefield                    Dubbeldam2007FlexibleIRMOF-1
EwaldPrecision                1e-6

Framework 0
FrameworkName IRMOF-1
UnitCells 3 3 3
ExternalTemperature 298.15
ComputeMSD yes
PrintMSDEvery 10

FrameworkDefinitions Dubbeldam2007FlexibleIRMOF-1

Component 0 MoleculeName              argon
            MoleculeDefinition        TraPPE
            MolFraction               0.10
            IdealGasRosenbluthWeight  1.0
            TranslationProbability    1.0
            RegrowProbability         0.5
            IdentityChangeProbability 1.0
              NumberofIdentityChanges 2
              IdentityChangeList      0 1
            RotationProbability       1.0
            ReinsertionProbability    1.0
            CreateNumberOfMolecules   16

Component 1 MoleculeName              methane
            MoleculeDefinition        TraPPE
            MolFraction               0.90
            IdealGasRosenbluthWeight  1.0
            TranslationProbability    1.0
            RegrowProbability         0.5
            IdentityChangeProbability 1.0
              NumberofIdentityChanges 2
              IdentityChangeList      0 1
            RotationProbability       1.0
            ReinsertionProbability    1.0
            CreateNumberOfMolecules   16
```