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SimulationType           MonteCarlo
NumberOfCycles           5000
NumberOfInitializationCycles 0
PrintEvery              1000
PrintPropertiesEvery    1000

Forcefield               Dubbeldam2007FlexibleIRMOF-1

Framework 0
FrameworkName IRMOF-1
RemoveAtomNumberCodeFromLabel yes
UnitCells 1 1 1
ExternalTemperature 573.0

Component 0 MoleculeName      C5
            MoleculeDefinition TraPPE
            IdealGasRosenbluthWeight 0.064
            WidomProbability     1.0
            CreateNumberOfMolecules 0

Component 1 MoleculeName      C6
            MoleculeDefinition TraPPE
            IdealGasRosenbluthWeight 0.0164423
            WidomProbability     1.0
            CreateNumberOfMolecules 0

Component 2 MoleculeName      C7
            MoleculeDefinition TraPPE
            IdealGasRosenbluthWeight 0.00425143
            WidomProbability     1.0
            CreateNumberOfMolecules 0

Component 3 MoleculeName      C8
            MoleculeDefinition TraPPE
            IdealGasRosenbluthWeight 0.0011068
            WidomProbability     1.0
            CreateNumberOfMolecules 0

Component 4 MoleculeName      C9
            MoleculeDefinition TraPPE
            IdealGasRosenbluthWeight 0.000289648
            WidomProbability     1.0
            CreateNumberOfMolecules 0

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