

SimulationType MolecularDynamics
NumberOfCycles 100000
NumberOfEquilibrationCycles 50000
NumberOfInitializationCycles 50000
PrintEvery 1000
RestartFile no

Ensemble NVT

Forcefield TraPPE
CutOff 12.0

Box 0

BoxLengths 30.0 30.0 30.0

ComputeRDF yes
WriteRDFEvery 10

RDFHistogramSize 300
RDFRange 15.0

ComputeMSD yes
PrintMSDEvery 10

ExternalTemperature 300.00

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